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Supplementary Information

Photochemistry of 1-phenyl-4-allyl-tetrazol-5-one: A Theoretical Study Contribution Towards Mechanism elucidation

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Abbreviations

- M—intermediate/minimum
- P—product
- S_0—ground state
- T_1—1st triplet state
- TS(a/0)—transition state (with bond break in ally/phenyl moiety)

A—Coordinates (z-matrix)

A.1—S_0 gas phase

Atom	Bond	B3LYP	M06HF	PBE0	Angle	B3LYP	M06HF	PBE0	Torsion	B3LYP	M06HF	PBE0
C												
C	1	1.39708	1.39258	1.39266								
C	1	1.39897	1.39486	1.39451	2	119.4261	119.5974	119.4372				
C	3	1.39504	1.39073	1.39046	1	120.6576	120.5871	120.6436	2	−0.0000	−0.0000	−0.0000
C	4	1.40305	1.39652	1.39789	3	119.2846	118.9091	119.2415	1	−0.0000	0.0000	−0.0000
C	2	1.39763	1.39393	1.39304	1	120.9206	120.9158	120.9180	5	−0.0000	0.0000	−0.0000
H	3	1.09248	1.08851	1.09172	4	119.1511	119.2010	119.1565	1	180.0000	180.0000	180.0000
H	1	1.09215	1.08828	1.09139	2	120.3327	120.2283	120.3239	3	−180.0000	−180.0000	−180.0000
H	2	1.09248	1.08846	1.09173	6	118.9422	118.9468	118.9428	1	180.0000	−180.0000	180.0000
H	6	1.08840	1.08689	1.08876	5	119.7372	119.7934	119.6421	2	180.0000	−180.0000	−180.0000
H	4	1.08911	1.08708	1.08910	5	119.6364	119.5351	119.5463	3	180.0000	180.0000	180.0000
N	5	1.42436	1.42113	1.41542	4	119.1252	118.7248	119.0689	3	−180.0000	−180.0000	−180.0000
N	12	1.37007	1.34956	1.35654	5	120.8219	121.1408	120.8432	4	1.1960	−4.2025	0.9031
C	12	1.39931	1.38189	1.39085	5	128.7598	128.5524	128.5872	4	−178.9528	174.5532	−179.1047
N	13	1.27140	1.24927	1.26478	12	108.8416	109.0238	108.8340	5	180.0000	178.9048	180.0000
N	15	1.35789	1.34026	1.34540	13	108.5653	108.7648	108.5252	12	0.0000	0.0000	0.0000
O	14	1.21949	1.21134	1.21510	12	130.9886	130.8844	131.1517	5	0.8924	1.3811	0.8862
C	16	1.45121	1.44663	1.44073	15	122.9055	123.0479	123.1311	13	−180.0000	−175.2471	−180.0000
C	18	1.50854	1.51514	1.50001	16	114.9854	112.6150	114.7229	15	77.7704	80.5221	76.1209
H	18	1.10319	1.09713	1.10209	16	108.0723	107.6885	108.3352	19	−123.7450	−122.4387	−123.9479
H	18	1.10237	1.09763	1.10179	20	107.4641	109.4973	107.4074	16	113.3984	114.6613	113.2837
C	19	1.33345	1.32766	1.33069	18	126.4313	124.4911	126.0583	16	−3.9781	−1.8340	−3.5213
H	22	1.09232	1.08928	1.09147	19	120.8446	120.7131	120.8416	18	180.0000	180.0000	180.0000
H	22	1.09274	1.09135	1.09247	23	117.1343	117.6620	117.2508	19	−180.0000	−180.0000	−180.0000
H	19	1.09661	1.09185	1.09559	22	119.9673	120.5522	120.0105	18	180.0000	−180.0000	180.0000

A.2—S_0 PCM (methanol)

Atom	Bond	B3LYP	M06HF	PBE0	Angle	B3LYP	M06HF	PBE0	Torsion	B3LYP	M06HF	PBE0
C												
C	1	1.39801	1.39377	1.39362								
C	1	1.39995	1.39622	1.39563	2	119.5047	119.6800	119.5177				
C	3	1.39588	1.39209	1.39142	1	120.5672	120.5334	120.5540	2	−0.0000	0.0000	−0.0000
C	4	1.40281	1.39678	1.39779	3	119.3375	118.9082	119.2948	1	0.0000	0.0000	0.0000
C	2	1.39834	1.39490	1.39386	1	120.8152	120.7686	120.8111	5	−0.0000	−0.0000	−0.0000
H	3	1.09232	1.08874	1.09171	4	119.1755	119.1903	119.1811	1	180.0000	180.0000	180.0000
H	1	1.09214	1.08858	1.09154	2	120.3139	120.2230	120.3097	3	−180.0000	−180.0000	−180.0000
H	2	1.09245	1.08877	1.09184	6	119.0325	119.0210	119.0285	1	180.0000	180.0000	180.0000
H	6	1.08815	1.08650	1.08841	5	119.9530	119.9718	119.8840	2	−180.0000	−180.0000	−180.0000
H	4	1.08946	1.08759	1.08952	5	119.8277	119.8815	119.7681	3	−180.0000	−180.0000	−180.0000
N	5	1.42528	1.42309	1.41634	4	119.0709	118.7613	119.0118	3	180.0000	180.0000	180.0000
N	12	1.36812	1.34733	1.35487	5	120.9136	121.1566	120.9333	4	−14.0501	−12.9834	−13.7065
C	12	1.39636	1.37913	1.38821	5	128.7817	128.6728	128.6111	4	165.0707	165.9403	165.4619
N	13	1.27283	1.25035	1.26604	12	108.6981	108.8828	108.6886	5	179.0625	178.9757	179.1307
N	15	1.35506	1.33798	1.34282	13	108.7150	108.9076	108.6885	12	−0.0000	0.0000	−0.0000
O	14	1.22350	1.21718	1.21893	12	130.5805	130.4097	130.7357	5	1711164	−175680	1234157
C	16	1.45497	1.45061	1.44413	15	122.7047	122.6512	122.9037	13	178.7444	−176.1842	180.0000
C	18	1.50777	1.51467	1.49941	16	114.9211	112.3298	114.6197	15	79.2191	83.1813	77.8626
H	18	1.10213	1.09660	1.10113	16	107.7939	107.4911	108.0347	19	−123.7538	−122.3359	−123.9116
H	18	1.10171	1.09717	1.10097	20	107.0978	109.0112	107.0522	16	113.3813	115.0187	113.3443
C	19	1.33463	1.32923	1.33197	18	126.5753	124.6674	126.1880	16	−4.4335	−0.0000	−4.0612
H	22	1.09270	1.08979	1.09198	19	120.7723	120.6385	120.7762	18	−180.0000	180.0000	−180.0000
H	22	1.09333	1.09225	1.09315	23	117.0539	117.5284	117.1563	19	−180.0000	−180.0000	−180.0000
H	19	1.09647	1.09200	1.09568	22	120.1223	120.6671	120.1838	18	180.0000	180.0000	180.0000

A.3—T_1 PCM (methanol)

Atom	Bond	B3LYP	M06HF	PBE0	Angle	B3LYP	M06HF	PBE0	Torsion	B3LYP	M06HF	PBE0
C												
C	1	1.39945	1.47248	1.39494								
C	1	1.39975	1.46727	1.39518	2	119.3973	119.2761	119.3912				
C	3	1.39491	1.34149	1.39080	1	120.6107	121.0073	120.5884	2	0.0000	−0.0000	0.0000
C	4	1.40725	1.48057	1.40151	3	119.5856	118.9815	119.5520	1	−0.0000	−0.0000	−0.0000
C	2	1.39625	1.34179	1.39206	1	120.9674	121.1502	120.9736	5	0.0000	0.0000	0.0000
H	3	1.09249	1.08898	1.09190	4	119.1894	120.1813	119.1848	1	−180.0000	180.0000	−180.0000
H	1	1.09207	1.08327	1.09148	2	120.2747	120.3562	120.2785	3	−180.0000	−180.0000	−180.0000
H	2	1.09242	1.08864	1.09184	6	118.8714	120.1005	118.8604	1	−180.0000	180.0000	−180.0000
H	6	1.08736	1.08630	1.08771	5	120.4866	122.5002	120.5647	2	180.0000	180.0000	180.0000
H	4	1.08932	1.08687	1.08952	5	119.4845	122.4126	119.4302	3	−180.0000	−180.0000	−180.0000
N	5	1.41580	1.38014	1.40810	4	118.0113	118.4324	117.9198	3	−180.0000	180.0000	−180.0000
N	12	1.36420	1.35450	1.35308	5	120.5804	121.6034	120.5152	4	18.0155	−6.7982	19.2294
C	12	1.41906	1.39363	1.40995	5	127.7912	128.9328	127.6907	4	−178.5745	172.5067	−180.0000
N	13	1.45975	1.25407	1.44033	12	103.9140	108.9564	103.8022	5	−170.7085	180.0000	−170.8057
N	15	1.36171	1.33568	1.35103	13	103.3476	109.0918	103.2083	12	−29.6337	0.0000	−31.7174
O	14	1.21031	1.21650	1.20497	12	129.1332	129.9572	129.3065	5	7.9735	0.0000	9.3258
C	16	1.45685	1.45141	1.44570	15	120.5465	122.5900	120.6615	13	−178.2239	−175.4638	−177.9061
C	18	1.50780	1.51481	1.49952	16	113.8330	112.2180	113.5104	15	85.6618	82.0806	85.3865
H	18	1.10453	1.09667	1.10360	16	108.1856	107.4636	108.3903	19	−123.0525	−122.3245	−123.0801
H	18	1.10132	1.09701	1.10071	20	107.2125	109.0189	107.1581	16	114.6041	114.9640	114.6519
C	19	1.33463	1.32919	1.33193	18	126.2146	124.6792	125.7390	16	0.0000	−1.6552	−0.0000
H	22	1.09279	1.08981	1.09206	19	120.8441	120.5919	120.8911	18	180.0000	180.0000	180.0000
H	22	1.09331	1.09222	1.09319	23	117.3018	117.4987	117.4365	19	−180.0000	180.0000	−180.0000
H	19	1.09621	1.09196	1.09532	22	120.2831	120.6161	120.3743	18	180.0000	180.0000	180.0000

A.4—**TS1a** PCM (methanol)

Atom	Bond	M06HF	Angle	M06HF	Torsion	M06HF
C						
C	**1**	1.43856				
C	**1**	1.43982	**2**	120.2318		
C	**3**	1.35214	**1**	120.5379	**2**	9.7145
C	**4**	1.48931	**3**	117.5813	**1**	8.5817
C	**2**	1.35199	**1**	120.8342	**5**	4.4925
H	**3**	1.09017	**4**	120.4995	**1**	175.7884
H	**1**	1.08543	**3**	119.5592	**2**	172.3464
H	**2**	1.09011	**6**	120.3051	**1**	−176.4087
H	**6**	1.08643	**2**	123.4874	**5**	−176.2236
H	**4**	1.09055	**3**	122.4673	**5**	178.3144
N	**5**	1.41551	**4**	114.1509	**3**	111.6262
N	**12**	1.29188	**5**	121.3974	**4**	5.4835
C	**12**	1.55419	**5**	126.5952	**4**	168.0765
N	**13**	1.11672	**12**	140.1384	**5**	168.3715
N	**14**	1.27806	**12**	108.8647	**5**	−169.9188
O	**14**	1.22781	**12**	112.6557	**5**	10.1498
C	**16**	1.44782	**14**	117.2257	**12**	176.5648
C	**18**	1.51775	**16**	112.9142	**14**	−102.7619
H	**18**	1.09935	**16**	109.1221	**19**	−120.5141
H	**18**	1.10277	**20**	108.0474	**16**	119.3535
C	**19**	1.33017	**18**	124.5736	**16**	3.1934
H	**22**	1.09040	**19**	121.1144	**18**	180.0000
H	**22**	1.09084	**23**	118.3871	**19**	−180.0000
H	**19**	1.09339	**22**	120.2300	**18**	−180.0000

A.5—**TS1p** PCM (methanol)

Atom	Bond	B3LYP	M06HF	PBE0	Angle	B3LYP	M06HF	PBE0	Torsion	B3LYP	M06HF	PBE0
C												
C	**1**	1.42266	1.41082	1.41941								
C	**1**	1.41667	1.40828	1.41369	**2**	120.3201	121.2472	120.3818				
C	**3**	1.37420	1.37186	1.36892	**1**	120.4830	119.7984	120.4216	**2**	0.0000	0.0000	0.0000
C	**4**	1.45520	1.44295	1.45115	**3**	119.8644	119.7809	119.8451	**1**	−1.0862	−0.0000	−1.1508
C	**2**	1.37255	1.37206	1.36727	**1**	121.0334	120.6105	120.9998	**5**	0.0000	0.0000	0.0000
H	**3**	1.09190	1.08802	1.09137	**4**	119.8366	120.3337	119.9085	**1**	−180.0000	−180.0000	−180.0000
H	**1**	1.09147	1.08831	1.09095	**3**	119.8714	119.3738	119.8421	**2**	−180.0000	180.0000	−180.0000
H	**2**	1.09213	1.08812	1.09161	**6**	119.6147	119.8324	119.6419	**1**	−180.0000	−180.0000	−180.0000
H	**6**	1.08810	1.08604	1.08845	**2**	122.1717	122.5731	122.2897	**5**	−180.0000	−180.0000	−180.0000
H	**4**	1.08960	1.08802	1.08982	**3**	122.3024	122.8017	122.3903	**5**	−178.6383	−180.0000	−178.8500
N	**5**	1.32394	1.31627	1.31581	**4**	117.4042	116.6265	117.3543	**3**	178.4842	180.0000	178.2371
N	**12**	1.70324	1.72139	1.70758	**5**	125.5407	128.5102	125.6941	**4**	−20.2904	−0.0000	−23.7765
C	**12**	1.41365	1.41254	1.40122	**5**	130.1978	129.0470	129.8213	**4**	172.7077	178.0919	172.5418
N	**13**	1.27047	1.25958	1.25681	**12**	101.8106	99.8570	101.5338	**5**	174.3035	156.3004	177.1240
N	**14**	1.36932	1.35236	1.36564	**12**	105.8816	105.9457	105.8876	**5**	172.6242	−173.3030	169.9654
O	**14**	1.23103	1.21601	1.22593	**12**	127.0486	126.9507	127.3416	**5**	−10.2075	6.5183	−13.3483
C	**16**	1.45378	1.44698	1.44370	**14**	122.8093	121.8474	122.3665	**12**	166.2847	164.8931	165.3684
C	**18**	1.51056	1.51757	1.50201	**16**	115.7095	113.7860	115.2631	**14**	−84.1940	−76.6207	−83.6580
H	**18**	1.10254	1.09727	1.10129	**16**	107.5984	107.4343	107.8242	**19**	−123.5771	−122.4705	−123.7172
H	**18**	1.10133	1.09739	1.10054	**20**	106.8133	108.5213	106.7563	**16**	113.8967	115.3742	113.9402
C	**19**	1.33512	1.32943	1.33248	**18**	126.5607	124.7096	126.1189	**16**	−6.0438	−2.4143	−4.7904
H	**22**	1.09305	1.09012	1.09217	**19**	120.8583	120.8503	120.8772	**18**	180.0000	180.0000	180.0000
H	**22**	1.09330	1.09214	1.09324	**23**	117.2197	117.8494	117.3023	**19**	−180.0000	−179.0140	−180.0000
H	**19**	1.09697	1.09268	1.09603	**22**	119.8534	120.4639	119.8971	**18**	180.0000	−180.0000	180.0000

A.6—**M0a** PCM (methanol)

Atom	Bond	M06HF	Angle	M06HF	Torsion	M06HF
C						
C	**1**	1.39631				
C	**1**	1.39492	**2**	120.0701		
C	**3**	1.39411	**1**	120.1009	**2**	−0.0000
C	**4**	1.39326	**3**	119.2039	**1**	0.8885
C	**2**	1.39350	**1**	120.2975	**5**	−0.0000
H	**3**	1.08857	**4**	119.5738	**1**	180.0000
H	**1**	1.08880	**3**	119.9521	**2**	−180.0000
H	**2**	1.08872	**6**	119.5107	**1**	180.0000
H	**6**	1.08819	**5**	119.8562	**2**	−180.0000
H	**4**	1.08945	**5**	119.7799	**3**	−180.0000
N	**5**	1.43560	**4**	118.8241	**3**	178.7955
N	**12**	1.38719	**5**	113.5958	**4**	−51.3347
C	**12**	1.39225	**5**	120.7917	**4**	122.2931
N	**13**	1.16448	**12**	128.6018	**5**	172.8213
N	**14**	1.40430	**12**	114.9486	**5**	180.0000
O	**14**	1.20608	**12**	121.2170	**5**	4.4894
C	**16**	1.44784	**14**	112.6425	**12**	146.9118
C	**18**	1.52083	**16**	112.3575	**14**	−72.4259
H	**18**	1.09600	**16**	108.4161	**19**	−121.9348
H	**18**	1.10161	**20**	109.5958	**16**	117.6768
C	**19**	1.33091	**18**	125.2446	**16**	−10.2470
H	**22**	1.08997	**19**	120.4772	**18**	180.0000
H	**22**	1.09174	**23**	117.3227	**19**	−178.7568
H	**19**	1.09181	**22**	120.1758	**18**	180.0000

A.7—**M0p** PCM(methanol)

Atom	Bond	B3LYP	M06HF	PBE0	Angle	B3LYP	M06HF	PBE0	Torsion	B3LYP	M06HF	PBE0
C												
C	**1**	1.40849	1.40554	1.40374								
C	**1**	1.40696	1.40362	1.40226	**2**	120.3268	120.8175	120.3971				
C	**3**	1.38454	1.37697	1.38074	**1**	119.9624	119.3028	119.9123	**2**	0.0000	−0.0000	0.0000
C	**4**	1.43426	1.43816	1.42816	**3**	120.7994	121.3300	120.7333	**1**	−0.0000	−0.0000	−0.0000
C	**2**	1.38389	1.37907	1.37995	**1**	120.5937	120.9133	120.5296	**5**	0.0000	−0.0000	0.0000
H	**3**	1.09192	1.08829	1.09130	**4**	120.1393	120.5002	120.1636	**1**	−180.0000	−180.0000	−180.0000
H	**1**	1.09224	1.08882	1.09176	**2**	119.8636	119.4780	119.8475	**3**	−180.0000	180.0000	−180.0000
H	**2**	1.09229	1.08854	1.09167	**6**	119.7657	119.6271	119.8095	**1**	180.0000	180.0000	180.0000
H	**6**	1.08965	1.08432	1.08980	**2**	120.6346	121.2610	120.6785	**5**	180.0000	180.0000	179.1870
H	**4**	1.09150	1.08877	1.09115	**5**	121.5914	116.4840	117.6006	**3**	180.0000	180.0000	180.0000
N	**5**	1.34535	1.33313	1.33999	**4**	116.6778	114.0645	116.7302	**3**	178.2469	−180.0000	178.2255
N	**12**	2.66840	2.64440	2.64387	**5**	124.4435	149.3674	123.6735	**4**	−79.4801	−11.6686	−80.1483
C	**12**	1.37995	1.38334	1.37429	**5**	121.8553	121.9325	121.3541	**4**	169.6813	177.7650	170.1993
N	**13**	1.18453	1.16796	1.18235	**12**	84.2223	82.9960	84.0677	**5**	−137.6113	−175.8107	−136.7164
N	**15**	1.40465	1.37836	1.38128	**13**	127.1451	128.8838	127.3535	**12**	6.2077	6.1719	7.3713
O	**14**	1.22870	1.21705	1.22297	**12**	125.5919	128.5673	125.5043	**5**	−47.1954	−5.4345	−48.9359
C	**16**	1.46383	1.45637	1.45305	**15**	113.6057	113.2666	114.0239	**13**	176.5210	−176.6258	176.8679
C	**18**	1.50784	1.51634	1.49940	**16**	114.6304	112.4943	114.3660	**15**	88.8745	85.1881	87.9278
H	**18**	1.10128	1.09665	1.10036	**16**	107.1343	107.1961	107.2034	**19**	−122.5386	−121.2869	−122.6681
H	**18**	1.09961	1.09446	1.09913	**20**	107.2327	109.1403	107.2057	**16**	114.9500	116.1910	114.8973
C	**19**	1.33527	1.32999	1.33260	**18**	126.2535	124.4317	125.8443	**16**	−1.7135	−1.9886	−1.5476
H	**22**	1.09281	1.09000	1.09208	**19**	120.9893	120.8145	120.9931	**18**	−180.0000	−180.0000	−180.0000
H	**22**	1.09389	1.09260	1.09374	**23**	117.1556	117.5936	117.2273	**19**	180.0000	−180.0000	180.0000
H	**19**	1.09685	1.09242	1.09595	**22**	119.9312	120.5045	119.9816	**18**	180.0000	180.0000	180.0000

A.8—**TS2a** PCM(methanol)

Atom	Bond	M06HF	Angle	M06HF	Torsion	M06HF
C						
C	**1**	1.39444				
C	**1**	1.39813	**2**	120.2979		
C	**3**	1.39165	**1**	120.0799	**2**	0.0000
C	**4**	1.39691	**3**	119.1588	**1**	−0.0000
C	**5**	1.39204	**4**	121.2019	**3**	0.0000
H	**3**	1.08866	**4**	119.7350	**1**	−180.0000
H	**1**	1.08897	**2**	119.8806	**3**	−180.0000
H	**2**	1.08856	**6**	119.8422	**1**	−180.0000
H	**6**	1.08876	**5**	119.1136	**2**	−180.0000
H	**4**	1.08969	**5**	119.8155	**3**	180.0000
N	**5**	1.43117	**4**	120.8227	**3**	178.5261
N	**12**	1.57780	**5**	110.0643	**4**	−83.5784
C	**12**	1.39287	**5**	118.9775	**4**	54.1692
N	**13**	1.13178	**12**	122.7204	**5**	−156.5641
N	**14**	1.40956	**12**	114.8433	**5**	−160.3593
O	**14**	1.20729	**12**	121.2601	**5**	25.8800
C	**16**	1.44735	**14**	112.2531	**12**	150.9090
C	**18**	1.52113	**16**	112.6251	**14**	−75.0099
H	**18**	1.09614	**16**	108.4783	**19**	−121.6626
H	**18**	1.10149	**20**	109.7171	**16**	117.8337
C	**19**	1.33116	**18**	125.5789	**16**	−11.4609
H	**22**	1.09005	**19**	120.3927	**18**	−180.0000
H	**22**	1.09110	**23**	117.3155	**19**	−179.1293
H	**19**	1.09189	**22**	120.1404	**18**	178.9645

A.9—**TS2p** PCM(methanol)

Atom	Bond	B3LYP	M06HF	PBE0	An-gle	B3LYP	M06HF	PBE0	Torsion	B3LYP	M06HF	PBE0
C												
C	**1**	1.40818	1.40504	1.40308								
C	**1**	1.40632	1.40272	1.40161	**2**	120.2632	120.7723	120.3294				
C	**3**	1.38491	1.37916	1.38139	**1**	120.0120	119.5476	119.9819	**2**	0.0000	0.0000	0.0000
C	**4**	1.43334	1.43278	1.42651	**3**	120.8230	120.9235	120.7178	**1**	0.0000	−0.0000	0.0000
C	**2**	1.38485	1.37947	1.38120	**1**	120.5726	120.6242	120.4715	**5**	0.0000	0.0000	0.0000
H	**3**	1.09206	1.08841	1.09147	**4**	120.1078	120.3522	120.1188	**1**	−180.0000	−180.0000	−180.0000
H	**1**	1.09217	1.08888	1.09166	**3**	119.8699	119.6856	119.8238	**2**	−180.0000	−180.0000	−180.0000
H	**2**	1.09228	1.08861	1.09158	**6**	119.7485	119.8087	119.7705	**1**	180.0000	180.0000	180.0000
H	**6**	1.09020	1.08696	1.09062	**2**	120.6301	120.9366	120.6483	**5**	180.0000	180.0000	180.0000
H	**4**	1.09157	1.08872	1.09126	**5**	117.5562	117.0008	117.6254	**3**	−180.0000	−180.0000	−180.0000
N	**5**	1.34619	1.33332	1.34158	**4**	116.7070	115.8348	116.9220	**3**	177.6623	177.7563	177.8320
N	**12**	2.73155	2.75363	2.72328	**5**	123.7537	131.5164	119.7510	**4**	−74.8034	−66.3764	−77.8619
C	**12**	1.38618	1.39234	1.38166	**5**	121.5192	120.3395	120.8273	**4**	171.9887	174.2835	172.6678
N	**13**	1.14904	1.12336	1.13963	**12**	83.9910	79.1400	83.2026	**5**	−141.6940	−155.2345	−141.7028
N	**14**	1.39110	1.38993	1.38362	**12**	115.5618	114.5409	115.8191	**5**	129.1483	140.0471	122.8421
O	**14**	1.23191	1.21510	1.22595	**12**	124.4911	125.4279	123.9475	**5**	−53.7453	−41.3316	−59.0674
C	**16**	1.45596	1.45469	1.44507	**14**	121.7127	118.8992	120.6476	**12**	160.7939	152.3348	156.8017
C	**18**	1.50890	1.51569	1.50022	**16**	116.4954	114.4703	116.5040	**14**	−76.4881	−68.7584	−72.3778
H	**18**	1.10242	1.09733	1.10164	**16**	107.2352	107.4371	107.4479	**19**	−123.3583	−122.7411	−123.7598
H	**18**	1.10122	1.09763	1.10130	**20**	106.3482	108.3019	106.1041	**16**	113.8009	114.5382	113.5667
C	**19**	1.33564	1.33009	1.33315	**18**	126.6487	125.1209	126.3219	**16**	−3.5457	0.9659	−3.0177
H	**22**	1.09298	1.09011	1.09220	**19**	120.9185	120.7036	120.9500	**18**	−180.0000	180.0000	−180.0000
H	**22**	1.09386	1.09278	1.09392	**23**	116.8981	117.3931	116.9414	**19**	180.0000	−180.0000	180.0000
H	**19**	1.09737	1.09281	1.09644	**22**	119.6324	120.1488	119.6439	**18**	179.0099	−180.0000	179.0982

A.10—**M1** PCM(methanol)

Atom	Bond	B3LYP	M06HF	PBE0	Angle	B3LYP	M06HF	PBE0	Torsion	B3LYP	M06HF	PBE0
C												
C	**1**	1.40813	1.40469	1.40342								
C	**1**	1.40645	1.40281	1.40182	**2**	120.2990	120.7443	120.3583				
C	**3**	1.38462	1.37895	1.38085	**1**	119.8878	119.4873	119.8258	**2**	0.0000	−0.0000	0.0000
C	**4**	1.43391	1.43280	1.42801	**3**	120.9488	121.0360	120.9060	**1**	0.0000	0.0000	0.0000
C	**2**	1.38501	1.38007	1.38110	**1**	120.6719	120.6961	120.6190	**5**	−0.0000	−0.0000	−0.0000
H	**3**	1.09214	1.08821	1.09152	**4**	120.1147	120.2491	120.1374	**1**	180.0000	180.0000	180.0000
H	**1**	1.09227	1.08893	1.09184	**3**	119.8657	119.6043	119.8375	**2**	180.0000	180.0000	180.0000
H	**2**	1.09214	1.08856	1.09158	**6**	119.6472	119.7331	119.6728	**1**	−180.0000	−180.0000	−180.0000
H	**6**	1.08893	1.08610	1.08905	**2**	120.8390	120.8813	120.8362	**5**	−180.0000	−180.0000	−180.0000
H	**4**	1.09164	1.08873	1.09136	**5**	121.5131	117.0041	117.5253	**3**	180.0000	−180.0000	−180.0000
N	**5**	1.34887	1.33684	1.34368	**4**	116.2714	115.4071	116.2886	**3**	−178.1279	−178.8783	−178.3279
C	**12**	1.38473	1.39003	1.37964	**5**	123.4014	121.3905	122.6035	**4**	−170.8448	−172.4151	−169.9662
N	**13**	1.39480	1.41006	1.39096	**12**	110.7796	111.2808	110.9205	**5**	−148.6250	−152.9738	−147.8753
O	**13**	1.23385	1.21295	1.22734	**12**	127.2625	127.1237	127.1759	**5**	31.2658	26.7580	31.9587
C	**14**	1.44668	1.45036	1.43676	**13**	117.3206	114.0210	116.5458	**12**	−136.0542	−133.5104	−134.5307
C	**16**	1.51690	1.52042	1.50747	**14**	112.4286	112.0414	112.8908	**13**	98.1336	80.5974	89.0256
H	**16**	1.10730	1.10242	1.10713	**14**	110.5536	108.4730	109.5476	**17**	−122.3614	−120.1712	−121.4113
H	**16**	1.10476	1.09662	1.10249	**18**	107.8412	109.4488	107.9258	**14**	118.4181	118.3968	118.4975
C	**17**	1.33645	1.33116	1.33380	**16**	125.9711	125.0711	125.8078	**14**	−7.9542	−0.0000	−4.3524
H	**20**	1.09321	1.09041	1.09250	**17**	120.7167	120.2317	120.6290	**16**	−180.0000	180.0000	180.0000
H	**20**	1.09340	1.09141	1.09343	**21**	117.5721	117.9567	117.6713	**17**	−180.0000	−180.0000	−180.0000
H	**17**	1.09625	1.09233	1.09567	**20**	120.3814	120.5487	120.3861	**16**	−180.0000	−180.0000	−179.1510

A.11—**TS3** PCM(methanol)

Atom	Bond	B3LYP	M06HF	PBE0	Angle	B3LYP	M06HF	PBE0	Torsion	B3LYP	M06HF	PBE0
C												
C	**1**	1.40208	1.39789	1.39785								
C	**1**	1.40111	1.39658	1.39685	**2**	119.6890	119.9944	119.7484				
C	**3**	1.39419	1.39126	1.38951	**1**	120.1529	119.9559	120.0986	**2**	−0.0000	−0.0000	−0.0000
C	**4**	1.41303	1.40434	1.40874	**3**	120.6085	120.2749	120.6082	**1**	−0.0000	−0.0000	−0.0000
C	**2**	1.39394	1.39111	1.38949	**1**	120.6030	120.4418	120.5878	**5**	−0.0000	−0.0000	−0.0000
H	**3**	1.09268	1.08894	1.09202	**4**	119.7528	119.8970	119.8002	**1**	180.0000	−180.0000	180.0000
H	**1**	1.09243	1.08901	1.09187	**3**	120.1510	120.0169	120.1281	**2**	−180.0000	−180.0000	−180.0000
H	**2**	1.09280	1.08897	1.09214	**6**	119.4694	119.5327	119.5020	**1**	180.0000	180.0000	180.0000
H	**6**	1.09001	1.08856	1.09007	**2**	120.3508	120.6248	120.4352	**5**	179.0683	180.0000	179.0339
H	**4**	1.09232	1.08940	1.09194	**5**	118.5946	118.3457	118.4538	**3**	180.0000	180.0000	180.0000
N	**5**	1.39650	1.39952	1.38659	**4**	117.3857	116.7212	117.1586	**3**	178.5198	178.1451	178.4057
C	**12**	1.36801	1.37857	1.36431	**5**	122.9875	120.1073	122.6617	**4**	152.7518	155.2295	155.3760
N	**13**	1.41640	1.42296	1.40998	**12**	116.5825	113.8826	115.8827	**5**	161.7315	153.6162	158.9616
O	**13**	1.23494	1.21154	1.22816	**12**	126.0869	126.2148	126.1916	**5**	−25.1035	−30.6541	−28.0624
C	**14**	1.46060	1.46539	1.44882	**13**	113.9493	109.6421	113.1903	**12**	−68.4295	−78.2222	−71.5551
C	**16**	1.50792	1.51626	1.50086	**14**	111.1987	108.0420	110.5837	**13**	42.2903	49.9256	45.6152
H	**16**	1.10911	1.10262	1.10790	**14**	108.1622	108.2682	108.3703	**17**	−121.2288	−119.2819	−120.9457
H	**16**	1.10589	1.09759	1.10447	**18**	106.1026	108.7674	106.1337	**14**	115.9389	118.2259	116.7114
C	**17**	1.37775	1.36054	1.36857	**16**	118.0475	118.4401	118.1954	**14**	33.1756	34.6826	32.7381
H	**20**	1.09263	1.09074	1.09246	**17**	120.5595	120.7080	120.8079	**12**	−108.3519	−104.5963	−107.8274
H	**20**	1.09122	1.08962	1.09126	**21**	115.7913	117.2585	116.1084	**17**	160.2017	167.8584	163.0546
H	**17**	1.09318	1.08960	1.09279	**20**	121.0391	121.3267	121.1171	**16**	167.1692	170.8587	168.7151

A.12—**M2** PCM(methanol)

Atom	Bond	B3LYP	M06HF	PBE0	Angle	B3LYP	M06HF	PBE0	Torsion	B3LYP	M06HF	PBE0
C												
C	**1**	1.39882	1.39560	1.39445								
C	**1**	1.39855	1.39417	1.39403	**2**	119.2632	119.4489	119.2364				
C	**3**	1.39689	1.39448	1.39259	**1**	120.4539	120.4008	120.4464	**2**	−0.0000	−0.8386	−0.0000
C	**4**	1.40730	1.39929	1.40237	**3**	120.3272	119.9447	120.3264	**1**	0.0000	0.9754	0.0000
C	**2**	1.39722	1.39339	1.39288	**1**	120.8720	120.7067	120.9062	**4**	−0.0000	−0.0000	−0.0000
H	**3**	1.09258	1.08894	1.09197	**4**	119.2799	119.3165	119.2638	**1**	180.0000	179.1204	180.0000
H	**1**	1.09230	1.08876	1.09167	**3**	120.3337	120.2443	120.3551	**2**	−180.0000	−180.0000	−180.0000
H	**2**	1.09289	1.08909	1.09229	**6**	119.0804	119.1676	119.0499	**1**	180.0000	180.0000	180.0000
H	**6**	1.08690	1.08605	1.08694	**5**	119.5836	119.5505	119.5399	**2**	−180.0000	−180.0000	−180.0000
H	**4**	1.09081	1.08925	1.09078	**3**	119.2500	119.8104	119.2684	**5**	−179.1540	−180.0000	−179.1889
N	**5**	1.42592	1.42280	1.41683	**4**	119.3334	119.1245	119.2270	**3**	178.6391	178.6025	178.6602
C	**12**	1.38316	1.36212	1.37488	**5**	121.8446	121.5486	121.8547	**4**	140.2324	138.8457	141.2093
N	**13**	1.39895	1.41802	1.39459	**12**	116.6226	114.8867	116.2466	**5**	−164.8822	−169.9378	−164.6265
O	**13**	1.23252	1.21550	1.22650	**12**	124.6463	125.5923	124.8917	**5**	11.7172	7.7437	11.9407
C	**14**	1.44887	1.45554	1.43866	**13**	116.1222	113.1299	115.8497	**12**	−48.7490	−54.7026	−49.9283
C	**16**	1.49465	1.50631	1.48820	**14**	111.6275	109.3273	111.3295	**13**	42.3145	51.3803	43.3576
H	**16**	1.11601	1.10762	1.11426	**14**	108.2003	108.2054	108.3238	**17**	−122.7069	−120.4635	−122.5862
H	**16**	1.10728	1.09742	1.10559	**18**	104.8165	108.0078	104.8898	**14**	115.6836	117.5000	115.9665
C	**12**	1.47903	1.47223	1.46685	**5**	118.6476	119.7489	118.6827	**4**	−32.3074	−35.0415	−31.1501
H	**20**	1.09989	1.09533	1.09927	**12**	107.8741	107.7427	107.8760	**17**	121.0374	119.7615	120.7924
H	**20**	1.11194	1.10449	1.11074	**21**	106.5310	108.6287	106.5614	**12**	−118.1924	−119.2173	−118.5173
H	**17**	1.09155	1.08612	1.09071	**20**	119.3980	119.7786	119.4761	**16**	−162.7544	−157.7899	−162.1311

A.13—**TS4** PCM (methanol)

Atom	Bond	B3LYP	M06HF	PBE0	Angle	B3LYP	M06HF	PBE0	Torsion	B3LYP	M06HF	PBE0
C												
C	**1**	1.40034	1.39689	1.39599								
C	**1**	1.39718	1.39292	1.39284	**2**	119.2130	119.4022	119.2044				
C	**3**	1.39921	1.39564	1.39469	**1**	120.4625	120.3686	120.4502	**2**	−0.0000	−0.8682	−0.0000
C	**4**	1.40486	1.39816	1.40015	**3**	120.3754	120.1027	120.3724	**1**	0.0000	0.0000	0.0000
C	**2**	1.39602	1.39205	1.39167	**1**	120.7608	120.6808	120.7815	**4**	−0.0000	0.0000	0.0000
H	**3**	1.09275	1.08904	1.09214	**4**	119.2470	119.3166	119.2429	**1**	180.0000	180.0000	180.0000
H	**1**	1.09239	1.08877	1.09176	**3**	120.3939	120.3038	120.3921	**2**	−180.0000	−180.0000	−180.0000
H	**2**	1.09295	1.08912	1.09233	**6**	119.1375	119.2353	119.1209	**1**	180.0000	180.0000	180.0000
H	**6**	1.08842	1.08647	1.08835	**5**	120.1372	119.5108	120.2338	**2**	180.0000	−180.0000	180.0000
H	**4**	1.09097	1.08883	1.09089	**3**	119.2740	119.6678	119.3102	**5**	−180.0000	−180.0000	−180.0000
N	**5**	1.43080	1.42681	1.42117	**4**	119.6636	119.1290	119.5656	**3**	177.5734	177.8012	177.6148
C	**12**	1.39080	1.37540	1.38385	**5**	120.3125	119.7872	120.1809	**4**	136.5952	135.2019	136.8847
N	**13**	1.42262	1.41932	1.41306	**12**	120.2558	119.9445	120.1747	**5**	−178.7638	−175.6387	−177.9126
O	**13**	1.23041	1.21741	1.22563	**12**	122.3936	122.4755	122.3317	**5**	1.1896	3.4974	1.7559
C	**14**	1.45024	1.42821	1.43872	**13**	118.3447	118.1076	118.2484	**12**	0.0000	−3.2902	−0.0000
C	**16**	1.46646	1.47407	1.46155	**14**	116.4939	116.5496	116.5445	**13**	−20.9215	−20.9667	−20.9372
H	**16**	1.09305	1.08893	1.09242	**14**	113.4763	114.1828	113.6394	**17**	−152.1300	−153.7369	−152.9345
H	**14**	1.23236	1.23586	1.22784	**16**	59.0789	60.1492	58.8565	**18**	89.5828	90.6975	89.5837
C	**12**	1.48852	1.48136	1.47853	**5**	113.6381	116.7239	116.8513	**4**	46.8748	−38.4289	−36.0695
H	**20**	1.09775	1.09477	1.09752	**12**	107.5475	107.1452	107.6009	**17**	121.3317	120.6581	121.2533
H	**20**	1.10661	1.10092	1.10590	**21**	108.0954	109.6657	108.0593	**12**	−118.6040	−119.7388	−119.0574
H	**17**	1.09720	1.09152	1.09651	**16**	118.6272	118.4114	118.5354	**20**	−148.0472	−144.5677	−146.9905

A.14—**P(T_1)** PCM(methanol)

Atom	Bond	B3LYP	M06HF	PBE0	Angle	B3LYP	M06HF	PBE0	Torsion	B3LYP	M06HF	PBE0
C												
C	1	1.44421	1.35070	1.44441								
C	1	1.46951	1.44662	1.46524	2	118.8387	119.9801	118.8059				
C	3	1.35657	1.42313	1.35193	1	120.8002	120.6991	120.7688	2	−2.0873	12.2280	−1.9797
C	4	1.46718	1.37122	1.46279	3	120.7688	119.6616	120.7166	1	1.2830	−11.7336	1.3376
C	2	1.35903	1.48685	1.35344	1	121.5579	117.4226	121.4365	4	−0.0000	16.5350	−0.0000
H	3	1.09231	1.08622	1.09168	4	120.0374	119.0015	120.0235	1	−178.9204	−169.4648	−178.9060
H	1	1.08992	1.09067	1.08926	3	120.8116	121.1322	120.8036	2	180.0000	175.6577	180.0000
H	2	1.09346	1.08989	1.09263	6	119.4883	122.1424	119.5594	1	−179.1208	175.4058	−178.9136
H	6	1.08709	1.09812	1.08745	5	121.3035	113.6262	121.2830	2	177.9065	−139.0152	178.1479
H	4	1.09142	1.08926	1.09138	3	119.8581	121.6401	119.8936	5	176.5732	−175.3402	176.4963
N	5	1.38499	1.39382	1.38006	4	120.8336	123.0095	120.6430	3	−174.9128	177.9193	−174.5518
C	12	1.40790	1.38617	1.39727	5	120.2589	119.2226	119.9265	4	−147.8068	−155.6804	−147.5629
N	13	1.38013	1.36798	1.37262	12	115.4230	115.3691	115.4108	5	−165.7620	−170.8577	−166.7703
O	13	1.23392	1.21922	1.22811	12	122.8063	123.2077	122.8134	5	12.2061	8.3763	11.4383
C	14	1.39308	1.39530	1.38639	13	124.3603	123.7763	124.0868	12	3.1574	5.7059	4.6711
C	16	1.33979	1.32913	1.33629	14	120.2546	120.3947	120.2369	13	−12.6720	−15.1139	−13.9606
C	12	1.48934	1.47038	1.47546	5	119.1468	118.3151	119.1122	4	25.3083	13.5417	25.1112
H	14	1.01397	1.01288	1.01229	13	114.7520	114.9297	114.7212	16	172.4360	170.8934	170.6928
H	16	1.09039	1.08758	1.08990	14	115.6423	115.5030	115.7677	17	180.0000	180.0000	180.0000
H	18	1.10897	1.10319	1.10815	12	109.0665	110.0307	109.4426	17	123.1080	123.3801	123.1548
H	18	1.09880	1.09634	1.09850	21	107.0153	108.2293	106.9697	12	−115.8199	−116.4098	−115.9847
H	17	1.08975	1.08692	1.08906	16	121.3627	121.4051	121.3158	18	−178.4698	−179.0746	−178.5526

A.15—**P(S_0)** PCM (methanol)

Atom	Bond	B3LYP	M06HF	PBE0	Angle	B3LYP	M06HF	PBE0	Torsion	B3LYP	M06HF	PBE0
C												
C	1	1.40061	1.39752	1.39621								
C	1	1.39639	1.39162	1.39200	2	119.0977	119.2614	119.0622				
C	3	1.39991	1.39695	1.39552	1	120.5715	120.5250	120.5844	2	0.0000	0.0000	0.0000
C	4	1.40565	1.39871	1.40111	3	120.4509	120.1537	120.4521	1	−0.0000	−0.0000	−0.0000
C	2	1.39552	1.39115	1.39113	1	120.7910	120.7100	120.8265	4	0.0000	0.0000	0.0000
H	3	1.09281	1.08909	1.09217	4	119.1536	119.1835	119.1347	1	−180.0000	−180.0000	−180.0000
H	1	1.09239	1.08874	1.09175	3	120.4614	120.3748	120.4703	2	180.0000	180.0000	180.0000
H	2	1.09300	1.08916	1.09236	6	119.1017	119.1854	119.0635	1	−180.0000	−180.0000	−180.0000
H	6	1.08825	1.08646	1.08801	5	120.0873	119.4062	120.1501	2	−180.0000	180.0000	−180.0000
H	4	1.09042	1.08841	1.09035	3	119.0317	119.3670	119.0433	5	180.0000	180.0000	180.0000
N	5	1.42724	1.42208	1.41739	4	119.9656	119.7071	119.8929	3	−177.3000	−177.4247	−177.2393
C	12	1.39079	1.37508	1.38349	5	120.0796	119.6933	119.9925	4	−139.9154	−138.3170	−141.1148
N	13	1.38494	1.37483	1.37709	12	115.2469	115.2774	115.2072	5	−176.2464	−178.1011	−176.4703
O	13	1.23011	1.22145	1.22529	12	124.2495	124.0801	124.2311	5	2.5213	0.0000	2.3558
C	14	1.39704	1.39710	1.38948	13	123.4809	122.7975	123.3566	12	11.2442	14.3381	11.5958
C	16	1.33712	1.32932	1.33419	14	120.1549	119.9863	120.1055	13	−18.4176	−21.7766	−18.9580
C	12	1.48212	1.47158	1.46989	5	117.5522	117.7695	117.5086	4	28.4716	26.9412	26.6984
H	14	1.01393	1.01339	1.01227	13	113.9651	113.9166	113.8866	16	161.6079	159.1473	161.1468
H	16	1.09057	1.08782	1.09007	14	115.7039	115.6262	115.8024	17	180.0000	180.0000	180.0000
H	18	1.10997	1.10322	1.10915	12	110.3676	110.4053	110.5301	17	123.2629	122.1785	123.3302
H	18	1.10082	1.09601	1.10028	21	106.4486	108.3651	106.4520	12	−116.0612	−116.9499	−116.1263
H	17	1.08979	1.08680	1.08905	16	121.4782	121.7323	121.4491	18	−178.0273	−178.1326	−178.1504

A- Electronic Energy/Eh

	B3LYP	M06HF	PBE0
S0 gas	−680.9089562485	−681.1496384722	−680.5407704640
S0	−680.9179271575	−681.1612060994	−680.5502036252
T1	−680.8061598354	−681.0077792362	−680.4357080662
TS1a	-	−680.9010562926	-
TS1p	−680.7746150423	−680.9847053150	−680.3977906185
M0a	-	−681.0204322107	-
M0p	−680.8278283369	−681.0387611026	−680.4485953532
TS2a	-	−681.0147474125	-
TS2p	−680.8239372441	−681.0301883239	−680.4411875514
M1	−571.3904270865	−571.5700786161	−571.0733576913
TS3	−571.3644710498	−571.5497542036	−571.0515757600
M2	−571.4034505014	−571.6024479546	−571.0994514527
TS4	−571.3334454012	−571.5367107284	−571.0318774347
P(T_1)	−571.3903287049	−571.5899201828	−571.0847804355
P(S_0)	−571.5206313769	−571.7426664955	−571.2164418952

B- Harmonic Zero Point Energy/kJ mol^{-1}

	B3LYP	M06HF	PBE0
S0	507.942560	522.345595	513.988421
T1	499.725113	508.833783	506.157044
TS1a	-	498.950874	-
TS1p	489.870197	505.684579	494.853469
M0a	-	503.773358	-
M0p	493.021231	509.324366	498.842166
TS2a	-	497.901918	-
TS2p	486.728594	498.279037	491.508414
M1	467.861097	480.445609	472.293495
TS3	465.871760	478.414235	469.936951
M2	472.923602	485.160798	478.095819
TS4	461.094208	474.357444	467.354934
P(T_1)	476.412671	485.014426	471.369138
P(S_0)	486.181422	497.384915	491.514452

C- Vibrational Modes

D.1—**S_0** PCM (methanol)

B3LYP		M06HF		PBE0	
FREQ (cm^{-1})	**IR ITENS.**	**FREQ (cm^{-1})**	**IR ITENS.**	**FREQ (cm^{-1})**	**IR ITENS.**
8.651	0.000016	15.747	0.000332	10.097	0.000010
3.952	0.000160	8.974	0.001322	4.621	0.000172
2.794	0.000567	5.175	0.000164	4.120	0.001013
0.375	0.000020	2.289	0.000035	0.433	0.000011
0.240	0.000004	2.070	0.000069	0.221	0.000006
0.069	0.000002	0.340	0.000182	0.180	0.000005
43.506	0.023358	38.610	0.021036	42.469	0.022226
53.596	0.007621	47.398	0.008127	59.317	0.021365
66.390	0.041348	67.482	0.036082	69.016	0.029806
116.350	0.019976	121.294	0.042221	117.796	0.019902
135.344	0.025282	145.672	0.040120	143.117	0.034196
165.616	0.019771	172.564	0.015407	179.250	0.017150
212.144	0.098940	222.140	0.070065	215.436	0.092381
275.370	0.210559	284.590	0.237017	281.778	0.220898
300.272	0.142697	316.634	0.181764	305.088	0.153999
323.469	0.109870	329.964	0.091241	328.737	0.092381
329.492	0.058874	354.988	0.117194	334.424	0.072872
372.147	0.075777	371.782	0.066270	376.598	0.078874
429.350	0.007385	444.303	0.007331	430.718	0.007818

496.996	0.132916	517.749	0.192225	505.762	0.111454
527.400	0.335080	537.964	0.488138	531.141	0.409939
552.589	0.382359	562.411	0.517234	559.748	0.450484
625.202	0.015049	614.056	0.010419	622.944	0.012073
632.359	0.128288	641.560	0.525213	640.473	0.210824
676.304	0.124574	687.896	0.059888	685.318	0.118477
701.315	0.078121	727.398	0.909961	711.385	0.354129
715.100	0.585494	733.783	0.056057	720.534	0.521286
740.593	0.377465	785.753	0.271130	754.695	0.281297
769.814	0.474970	796.855	0.309630	782.144	1.005177
778.961	1.325352	808.885	2.630429	782.920	0.984660
814.946	0.558069	852.692	0.407203	835.223	0.476831
857.439	0.007396	897.046	0.002411	859.926	0.007439
924.091	0.181255	939.277	0.402898	940.838	0.363502
938.759	0.277145	981.486	0.001623	941.903	0.200941
939.257	0.619581	988.789	0.223062	945.838	0.878476
951.066	0.509398	1002.166	0.283314	967.011	0.282043
997.834	0.012819	1013.701	1.947287	1002.625	0.012576
1003.602	0.789432	1040.017	0.440643	1011.724	0.385307
1012.453	0.017180	1055.049	0.048553	1021.786	0.017505
1019.197	0.027111	1055.414	0.758562	1025.897	0.494860
1029.395	0.536533	1062.510	0.016642	1033.819	0.686216
1047.351	0.333027	1074.845	0.007854	1058.729	0.309944
1070.271	0.302212	1080.406	0.234637	1073.293	0.198113
1091.052	1.204662	1109.337	0.500938	1103.003	0.661922
1121.327	1.247698	1161.175	0.005759	1150.875	0.489803
1141.469	2.447629	1177.993	0.095239	1164.540	1.241170
1166.110	0.055022	1195.931	0.028225	1167.475	1.399748
1186.970	0.094647	1200.240	1.147728	1188.640	0.068036
1190.049	1.263349	1259.586	1.304128	1222.828	1.735264
1311.163	0.020436	1299.528	0.729349	1305.229	0.047861
1334.601	1.479546	1308.491	0.088237	1336.721	0.587293
1340.752	0.090854	1353.399	0.429564	1363.419	0.998368
1358.352	0.121709	1397.005	0.313251	1377.954	0.065305
1370.174	0.578325	1409.040	0.475143	1395.137	0.109859
1387.719	0.568516	1440.769	1.105928	1411.770	0.305846
1408.136	3.130984	1467.141	0.401625	1419.518	0.633380
1423.370	1.649535	1482.412	0.843247	1423.697	1.081063
1426.956	2.061619	1511.275	2.443259	1463.958	4.957352
1470.237	0.598385	1518.281	3.428520	1495.419	0.094888
1492.555	0.924369	1565.034	8.819812	1528.745	1.768581
1525.715	3.674942	1656.357	0.788176	1544.552	4.680320
1637.604	0.087884	1696.160	0.233405	1668.808	0.083478
1649.357	1.221118	1701.748	1.686166	1681.202	1.395794
1720.285	0.559180	1770.766	0.929408	1743.009	0.463296
1778.695	15.215420	1810.141	19.753581	1824.136	16.044662
3051.673	0.534597	3138.383	0.085702	3084.046	0.435644
3101.620	0.013348	3187.005	0.018531	3140.356	0.012597
3144.012	0.153956	3208.619	0.025698	3171.060	0.095630
3165.152	0.175524	3239.970	0.010250	3197.491	0.099176
3180.020	0.003095	3257.456	0.002939	3212.051	0.003709
3189.551	0.424103	3265.316	0.080849	3221.803	0.286630
3202.493	0.473522	3274.466	0.016552	3234.432	0.265057
3225.604	0.001848	3286.257	0.121478	3251.153	0.012967
3238.365	0.268268	3299.880	0.043248	3267.349	0.170147
3244.801	0.102905	3304.988	0.411429	3272.273	0.147196

D.2—$\mathbf{T_1}$ PCM (methanol)

B3LYP		M06HF		PBE0	
FREQ (cm^{-1})	**IR ITENS.**	**FREQ (cm^{-1})**	**IR ITENS.**	**FREQ (cm^{-1})**	**IR ITENS.**
14.137	0.008677	52.270	0.067519	17.709	0.010163
4.952	0.000511	13.581	0.000181	6.559	0.000307
2.869	0.001555	6.495	0.003920	2.914	0.001383
1.019	0.000062	2.189	0.000063	0.976	0.000073
0.328	0.000026	1.012	0.000031	0.433	0.000026
0.190	0.000009	0.313	0.000009	0.208	0.000009
37.490	0.023346	2.798	0.000470	39.260	0.014823
52.115	0.001149	36.654	0.024283	59.629	0.032239
59.335	0.030602	55.663	0.021912	62.904	0.009815
106.801	0.060105	70.721	0.063814	111.539	0.055495
119.587	0.030035	116.853	0.074368	121.755	0.045899
167.214	0.070066	147.126	0.037248	174.914	0.046686
191.190	0.143090	175.167	0.008169	194.457	0.143834
265.896	0.118589	194.934	0.004636	278.667	0.099114
281.996	0.423046	288.696	0.254710	290.822	0.380368
294.869	0.189193	306.925	0.119808	307.308	0.230986
317.343	0.109441	334.057	0.083621	326.567	0.264618
322.290	0.106648	349.068	0.145578	327.771	0.030753
373.274	0.003354	363.033	0.095911	380.752	0.014343
431.194	0.002430	410.908	1.400639	436.241	0.004768
494.137	0.264645	448.138	0.038219	502.189	0.235712
523.079	0.273380	516.652	0.209705	529.430	0.342276
554.057	0.413899	563.881	0.475483	564.515	0.502690
624.337	0.013936	568.990	0.005637	622.215	0.015705
643.864	0.416710	599.019	0.190160	650.506	0.476899
679.813	0.334896	608.187	0.273743	688.160	0.239969
693.112	0.508935	660.512	0.279211	706.669	0.499030
710.839	0.838622	718.261	0.054403	718.255	1.173308
727.684	0.238137	733.018	0.053047	739.673	0.295342
776.376	1.242473	757.885	2.434772	780.552	1.376530
779.680	0.047391	761.210	0.096825	798.932	0.010704
849.946	0.041201	776.782	0.554226	853.414	0.032490
871.081	0.137891	844.624	0.283243	899.524	0.304502
909.528	0.416471	870.084	0.676089	936.051	0.139818
932.672	0.132122	938.057	0.420039	942.014	0.814691
940.942	0.844353	957.396	0.116849	948.244	0.340296
952.123	0.157248	981.291	0.141755	976.052	0.212007
977.444	0.151172	1011.091	2.031242	999.169	0.065602
996.140	0.008845	1014.903	0.056439	1001.304	0.004329
1008.592	0.006247	1023.675	1.224144	1012.394	0.002840
1018.306	0.006188	1033.712	0.010861	1022.177	0.005852
1022.798	0.331803	1039.313	0.003248	1027.778	0.379439
1047.174	0.204460	1053.482	0.291626	1059.365	0.283133
1070.489	0.281305	1076.321	0.250705	1075.518	0.344750
1100.442	0.224397	1125.224	0.164763	1108.450	0.330008
1108.698	0.901357	1164.234	0.230780	1129.980	0.843437
1167.403	0.079562	1198.507	1.868632	1167.026	0.027727
1175.101	0.793843	1208.815	0.199119	1187.398	0.140045
1186.037	0.331654	1222.874	0.269073	1206.956	0.350768
1190.546	0.309670	1310.313	1.903748	1228.801	1.061635
1300.563	1.891870	1319.342	0.032706	1300.645	0.010518
1309.903	10.818088	1358.228	0.297044	1341.167	0.167145
1341.763	0.042407	1394.886	1.062640	1350.434	7.965323
1350.042	0.321406	1404.013	0.730813	1378.561	4.381824
1353.692	1.412412	1409.624	0.319007	1389.043	0.454761
1363.661	0.109035	1419.517	0.426221	1400.647	0.630494
1400.977	0.703330	1457.854	1.410724	1416.456	1.495000
1422.161	0.178990	1472.582	0.264253	1420.608	0.434418
1446.115	1.220088	1485.920	0.939884	1455.635	1.296845

1486.093	0.186154	1506.173	3.629189	1496.844	0.200750
1515.146	1.779018	1633.197	3.315061	1532.185	2.645501
1626.268	0.178233	1694.039	0.075449	1658.965	0.184279
1640.201	0.107190	1771.327	1.022862	1673.338	0.321090
1719.307	0.468853	1777.922	0.311458	1742.367	0.417576
1796.081	9.656169	1806.420	20.924261	1849.013	10.859863
3033.426	0.839218	3147.407	0.090798	3066.637	0.709425
3104.190	0.050673	3195.701	0.032210	3135.050	0.020841
3141.504	0.174754	3205.901	0.030009	3169.403	0.098178
3157.573	0.303535	3234.539	0.012435	3192.156	0.220248
3179.305	0.036861	3261.417	0.090374	3210.839	0.031661
3188.713	0.391726	3264.797	0.078384	3220.345	0.268024
3202.110	0.559754	3295.241	0.224111	3233.966	0.304994
3232.326	0.031234	3297.977	0.060831	3252.336	0.065510
3237.498	0.273638	3303.721	0.526453	3269.017	0.154526
3245.777	0.101013	3316.283	0.034250	3271.809	0.146717

D.3—**M0a** PCM (methanol)

M06HF	
FREQ (cm^{-1})	**IR ITENS.**
19.906	0.010460
16.465	0.014388
3.496	0.000635
1.301	0.000100
0.659	0.000020
2.847	0.001476
6.370	0.005716
21.170	0.033268
55.367	0.044841
75.289	0.060171
88.870	0.005707
105.744	0.008899
123.753	0.030742
168.437	0.055446
201.779	0.086962
272.796	0.192077
288.780	0.214373
332.282	0.190122
338.068	0.325425
405.552	0.004769
412.733	0.021471
430.818	0.107418
524.623	0.150612
554.219	0.711533
590.253	0.793602
606.678	0.950498
617.779	0.026117
670.570	1.261664
709.885	0.528598
718.682	1.559349
799.584	1.584931
809.407	0.956684
886.634	0.022961
894.779	0.060388
939.393	0.390776
979.811	0.052034
999.485	0.134394
1011.887	0.130736
1022.528	1.443160
1038.710	0.026418
1051.717	0.068139
1062.871	0.123430
1070.103	0.002981

1074.330	0.289800
1104.494	1.077627
1115.377	0.779927
1162.761	1.327923
1175.409	0.898584
1191.018	0.042529
1232.404	1.410410
1287.880	2.497605
1291.029	1.375409
1331.319	0.279169
1343.791	0.296042
1350.425	0.174578
1396.151	13.142107
1474.701	0.013136
1482.283	1.019482
1509.198	0.143452
1553.575	2.775801
1695.487	0.119658
1700.291	0.348070
1761.114	0.625035
1797.074	11.254312
1949.624	0.841780
3093.705	0.034140
3176.170	0.152015
3210.487	0.019388
3239.884	0.051148
3255.915	0.010045
3260.305	0.036061
3268.915	0.043554
3277.697	0.034579
3281.721	0.016338
3298.676	0.034842

D.4—**M0p** PCM (methanol)

B3LYP		**M06HF**		**PBE0**	
FREQ (cm^{-1})	**IR ITENS.**	**FREQ (cm^{-1})**	**IR ITENS.**	**FREQ (cm^{-1})**	**IR ITENS.**
20.183	0.019640	20.499	0.023499	15.366	0.019686
3.680	0.008568	5.009	0.008362	4.959	0.002999
3.109	0.006699	3.299	0.003230	3.202	0.006951
0.633	0.000016	0.832	0.000132	0.632	0.000012
0.430	0.000010	0.481	0.000024	0.505	0.000016
0.005	0.000001	0.434	0.000051	0.311	0.000003
30.765	0.080256	39.451	0.129662	32.825	0.089472
45.224	0.042157	53.108	0.003692	47.197	0.057537
56.629	0.037839	73.630	0.041001	59.141	0.031651
68.831	0.030524	99.529	0.026024	80.634	0.017727
90.973	0.026506	102.725	0.024833	95.253	0.028553
152.128	0.039841	141.964	0.059431	157.111	0.042312
168.432	0.091412	210.969	0.007568	175.716	0.098689
179.871	0.000573	235.204	0.026489	190.868	0.000055
213.665	0.103343	247.688	0.003425	224.768	0.095730
275.090	0.189812	261.211	0.021298	279.486	0.178395
289.463	0.011490	324.679	0.014846	297.489	0.014515
322.846	0.026837	336.684	0.014918	325.940	0.034869
350.791	0.141513	372.180	0.105547	350.153	0.146489
393.496	0.279883	399.385	0.325766	393.933	0.305772
421.117	0.924253	403.968	0.233820	426.773	0.916910
486.606	0.141066	506.122	0.038617	493.309	0.082619
493.592	0.292972	519.982	0.349165	503.232	0.393000
555.239	0.181020	566.356	0.138948	557.014	0.182106
568.664	0.474092	582.092	1.109697	571.642	0.349108
597.392	0.718739	590.829	0.060854	599.230	0.242369
612.437	1.138878	651.661	1.221271	625.695	1.366152

668.070	0.914541	677.396	1.323907	672.192	1.098346
707.900	0.382907	715.124	1.241832	716.029	1.058034
712.393	2.336437	768.084	0.876725	732.344	1.655290
793.189	1.801277	840.008	2.200086	800.625	1.460386
804.711	0.071679	852.050	0.643111	833.927	0.164722
832.308	0.139657	878.708	0.512605	842.004	0.277765
843.431	0.158311	881.832	0.052797	857.596	0.209512
904.712	1.732829	930.786	0.170972	927.937	0.584195
926.862	0.290289	973.437	0.258867	942.190	0.092748
948.019	1.524938	979.542	0.549034	953.492	1.634243
950.092	0.604709	1022.663	0.133990	955.685	1.010842
986.700	0.666687	1031.749	2.151173	992.235	0.557126
1001.406	0.015396	1049.884	0.086917	1006.195	0.018133
1020.650	0.024065	1059.499	0.181926	1022.013	0.031904
1027.419	0.046544	1066.592	0.048934	1034.135	0.191173
1031.538	0.038596	1070.669	1.245677	1046.904	0.017126
1047.306	1.765306	1088.104	0.029065	1058.801	0.669057
1074.913	1.370435	1127.612	0.522346	1101.345	2.363221
1105.017	0.583101	1136.015	4.441072	1115.815	0.832770
1124.624	6.568935	1165.411	0.884673	1144.037	8.249007
1160.152	0.040230	1172.980	7.733628	1160.930	0.163356
1182.261	0.010387	1212.893	3.542931	1194.555	0.485574
1271.288	11.706346	1297.943	0.711226	1291.898	5.814647
1307.280	0.054333	1315.007	0.014867	1305.155	0.064845
1312.726	0.700300	1324.070	8.609430	1319.988	0.527187
1331.146	6.306050	1341.417	0.807330	1349.831	7.938121
1353.073	0.574309	1390.956	13.740014	1379.764	0.989831
1381.729	2.588008	1419.410	3.853111	1389.054	2.675124
1401.315	2.746035	1448.912	6.531748	1407.838	0.323133
1418.774	0.646146	1468.287	0.203643	1418.697	0.802766
1426.438	1.955357	1482.554	0.873629	1436.077	7.032799
1462.135	0.420394	1489.466	1.241823	1476.107	0.529104
1479.730	0.683412	1502.064	2.112205	1492.986	1.139831
1564.326	0.110328	1609.525	0.347667	1591.656	0.096420
1604.418	3.962543	1641.284	10.155633	1629.813	4.620544
1668.504	10.417829	1753.991	12.576205	1721.289	11.111916
1717.913	0.441381	1772.762	1.108618	1741.091	0.611921
1782.565	1.462956	1930.347	1.883442	1823.201	1.406689
3060.238	0.571066	3156.909	0.195249	3089.499	0.435518
3113.683	0.028231	3202.666	0.041724	3148.244	0.019345
3135.720	0.433712	3205.828	0.003788	3164.502	0.219730
3147.171	0.233837	3232.208	0.094785	3180.963	0.257947
3185.703	0.005302	3268.110	0.036495	3216.557	0.006280
3195.386	0.144913	3278.916	0.016413	3227.496	0.088757
3204.080	0.301561	3283.101	0.011941	3234.054	0.137836
3213.378	0.230478	3293.117	0.064791	3244.388	0.146969
3226.981	0.030934	3293.195	0.097030	3253.014	0.035227
3234.010	0.328615	3329.800	0.580849	3268.259	0.193586

D.5- **M1** PCM (methanol)

B3LYP		M06HF		PBE0	
FREQ (cm^{-1})	**IR ITENS.**	**FREQ (cm^{-1})**	**IR ITENS.**	**FREQ (cm^{-1})**	**IR ITENS.**
18.422	0.006593	13.437	0.012931	13.687	0.009395
4.245	0.008413	6.125	0.006980	4.938	0.007003
1.553	0.006793	4.600	0.007477	3.299	0.008398
1.214	0.000499	2.187	0.000968	1.521	0.000187
0.830	0.000036	0.947	0.000061	0.703	0.000075
0.466	0.000012	0.528	0.000030	0.223	0.000003
31.083	0.063349	34.535	0.122803	27.730	0.038703
52.763	0.055670	54.424	0.065333	50.784	0.090445
60.319	0.070179	77.641	0.001335	74.423	0.047436
83.494	0.027717	102.227	0.104374	83.906	0.065971
149.759	0.039432	170.281	0.021324	153.170	0.019373
189.227	0.050996	190.928	0.009213	167.852	0.019168
214.670	0.111608	228.945	0.133107	216.160	0.154892
259.048	0.202672	276.398	0.215522	259.564	0.329395
296.697	0.695327	315.720	0.343549	302.141	0.514889
338.037	0.200928	351.843	0.305952	342.079	0.263273
381.449	0.164820	393.243	0.120619	385.135	0.146608
403.931	0.031946	406.349	0.022796	405.981	0.024282
494.128	0.063837	503.399	0.115738	494.012	0.089218
539.031	0.072244	562.264	0.626968	557.192	0.249230
573.513	0.730932	574.634	0.385783	568.682	0.479460
580.420	0.231031	588.295	0.202404	575.424	0.432279
608.290	0.017877	603.118	0.036944	607.936	0.010397
634.162	0.137485	654.402	0.541281	635.812	0.214288
667.395	0.981672	680.525	1.276529	671.446	1.159181
787.304	0.087115	804.266	0.139906	795.670	0.119449
797.657	1.185365	832.539	2.089651	804.032	1.294760
830.250	0.294639	853.132	0.427430	833.964	0.053051
835.878	0.010161	875.058	0.055822	845.302	0.262625
876.738	0.166012	897.074	0.137185	896.618	0.198739
918.653	0.169053	943.012	0.355887	940.238	0.103741
951.087	0.077036	976.424	1.477486	949.216	1.526204
952.666	1.428920	1011.855	0.949709	959.293	0.176112
989.289	0.543218	1015.068	0.358280	994.813	0.554727
999.259	0.016183	1037.763	1.692181	998.008	0.247430
1002.207	0.219838	1044.496	1.095856	1001.028	0.077774
1018.888	0.007733	1053.561	0.223539	1020.845	0.010972
1028.655	0.194407	1057.561	0.266544	1032.870	0.970235
1031.667	0.613631	1058.920	0.283998	1041.048	0.121431
1039.881	0.369443	1083.167	0.019791	1047.896	0.403046
1100.603	0.647225	1119.536	6.546741	1107.218	0.689504
1113.757	2.205766	1130.506	0.975406	1131.374	3.051131
1157.179	0.158150	1165.564	0.444945	1164.102	0.104516
1174.545	1.321734	1178.886	3.784930	1175.632	0.785389
1214.370	0.796770	1227.768	2.020904	1213.844	0.956138
1261.472	11.920549	1276.316	18.284591	1288.392	9.710438
1303.398	2.891947	1296.480	1.118626	1312.238	0.607189
1309.156	0.521651	1322.370	0.689008	1315.519	6.091443
1319.203	0.089023	1346.934	0.279453	1324.636	0.396264
1355.245	0.985881	1353.111	0.337694	1384.297	1.415528
1401.031	6.467915	1422.359	7.955727	1422.621	3.093118
1419.700	0.043752	1477.409	0.086901	1429.885	2.333559
1447.147	0.845847	1483.295	0.081107	1444.537	2.049091
1460.538	0.417754	1486.733	0.997542	1474.053	0.559454
1477.637	0.513273	1498.149	1.099118	1490.660	1.275948
1568.100	0.169651	1618.368	0.800809	1596.868	0.102768
1605.874	3.510906	1641.549	8.119648	1630.159	4.761982
1616.307	8.774813	1756.659	6.627554	1674.072	8.867038
1703.149	0.547886	1764.862	4.116181	1727.739	0.477599
2995.474	0.667485	3086.128	0.054780	3025.697	0.397549

3044.438	0.514150	3164.078	0.430434	3094.281	0.604820
3135.976	0.163636	3211.392	0.031779	3164.359	0.091903
3153.194	0.585726	3234.427	0.125685	3184.785	0.465694
3184.473	0.021092	3270.685	0.002623	3215.196	0.011884
3193.213	0.183256	3276.175	0.012566	3221.993	0.103774
3205.517	0.420416	3286.104	0.000733	3235.228	0.103264
3213.036	0.125392	3291.151	0.057084	3241.540	0.158975
3234.262	0.160403	3302.527	0.022570	3261.140	0.116661
3234.698	0.110207	3321.562	0.252717	3268.895	0.054187

D.6—**M2** PCM (methanol)

B3LYP		**M06HF**		**PBE0**	
FREQ (cm^{-1})	**IR ITENS.**	**FREQ (cm^{-1})**	**IR ITENS.**	**FREQ (cm^{-1})**	**IR ITENS.**
10.033	0.102423	14.870	0.206977	8.643	0.085971
7.875	0.000730	7.930	0.034140	7.314	0.020891
4.293	0.040454	3.191	0.004693	4.760	0.040474
0.753	0.000109	1.522	0.001043	1.377	0.000316
0.696	0.000065	0.877	0.000049	0.880	0.000030
0.266	0.000002	0.701	0.000213	0.239	0.000003
51.199	0.137481	53.148	0.067845	50.833	0.138789
88.971	0.009414	73.733	0.024522	90.346	0.010544
128.364	0.014125	106.416	0.010293	128.441	0.014469
156.357	0.098686	151.382	0.101732	157.861	0.101359
189.675	0.134319	186.541	0.339394	188.421	0.202736
223.390	0.183583	222.846	0.024971	220.522	0.157192
293.941	0.113809	294.174	0.017839	296.003	0.157070
296.678	0.030150	312.023	0.196178	299.435	0.008907
380.419	0.027309	384.255	0.147314	382.264	0.031660
413.505	0.723160	405.632	0.793765	416.631	0.774298
430.173	0.027942	445.339	0.053729	432.562	0.047194
502.801	0.559734	504.612	0.523384	504.296	0.603666
522.992	0.009589	535.281	0.153208	526.788	0.001225
538.306	0.041448	538.875	0.044442	541.648	0.045764
572.697	0.350439	594.133	0.532065	581.154	0.381971
626.280	0.048058	617.727	0.057520	624.030	0.055598
673.368	0.498494	671.622	0.620614	678.212	0.513091
710.228	0.932846	733.117	1.374483	715.062	1.163118
735.222	0.100579	766.830	0.148357	748.641	0.093956
774.407	0.785288	799.450	0.679936	777.695	0.948673
808.491	0.672136	821.601	1.558418	815.160	0.633079
840.520	0.025490	882.915	0.007312	844.642	0.026104
876.532	0.058730	893.153	0.062106	888.672	0.105061
920.468	0.089830	943.059	0.101544	923.817	0.100833
928.954	0.387477	960.360	0.198340	933.963	0.372632
949.779	0.193881	975.655	0.248431	962.983	0.057054
972.954	0.347146	993.914	0.321011	980.101	0.441933
984.755	0.051072	1006.517	0.030123	990.428	0.058270
1009.332	0.018180	1037.777	0.049244	1012.723	0.008979
1009.681	0.000792	1042.871	0.013714	1013.198	0.008987
1020.636	0.068803	1066.764	0.119070	1039.043	0.087861
1052.394	0.283898	1069.376	0.071093	1064.655	0.374428
1097.465	0.211118	1113.887	0.298636	1102.790	0.202005
1103.415	0.143723	1117.394	0.223531	1111.251	0.238752
1140.749	0.159425	1159.296	0.416569	1157.301	0.303920
1167.216	0.025766	1165.680	0.106206	1167.584	0.036713
1190.011	0.064412	1197.731	0.015376	1192.733	0.023972
1200.245	1.458111	1236.078	2.592957	1217.729	0.693752
1212.625	0.252759	1249.332	0.255137	1242.153	0.909885
1238.204	1.908598	1283.840	1.356168	1277.644	2.321884
1289.359	1.585929	1308.455	1.947871	1312.962	0.828770
1328.587	0.884553	1334.017	0.225998	1335.508	0.310943
1340.655	0.160345	1350.853	1.367679	1352.129	0.685649
1359.119	0.424769	1359.164	0.138184	1374.153	0.266468

1362.693	0.099059	1383.582	1.963603	1392.413	0.627137
1408.520	1.382176	1467.087	6.136141	1419.283	0.393845
1430.971	0.595900	1489.209	2.765341	1433.916	1.732286
1458.132	0.965956	1508.950	0.409869	1461.120	2.817786
1480.788	0.506581	1534.933	2.818968	1493.206	0.772798
1519.561	1.809774	1553.956	5.373196	1533.328	2.935517
1625.652	0.196523	1685.374	0.103346	1656.559	0.083304
1643.400	1.742000	1699.023	1.564412	1676.008	1.152915
1666.763	11.455040	1780.026	19.117960	1720.803	13.655990
2894.262	0.423384	3027.691	0.080995	2941.677	0.295186
2927.214	1.180810	3048.877	0.666131	2966.946	1.001215
3000.213	1.162256	3147.020	0.372095	3044.714	0.877261
3085.522	0.295112	3182.718	0.034873	3119.350	0.183476
3174.482	0.021877	3251.486	0.062861	3206.130	0.021704
3182.929	0.429469	3257.683	0.050949	3215.214	0.281935
3197.506	0.869530	3265.017	0.048098	3229.176	0.546998
3200.403	0.150564	3275.298	0.048465	3235.645	0.085934
3208.810	0.132248	3286.728	0.017064	3237.150	0.101792
3247.633	0.021875	3300.989	0.053662	3274.499	0.028442

D.7—**P(T_1)** PCM (methanol)

B3LYP		**M06HF**		**PBE0**	
FREQ (cm^{-1})	**IR ITENS.**	**FREQ (cm^{-1})**	**IR ITENS.**	**FREQ (cm^{-1})**	**IR ITENS.**
13.092	0.052233	11.300	0.045002	15.413	0.048698
7.923	0.023148	4.196	0.021985	9.505	0.033475
4.003	0.018319	1.858	0.034304	4.824	0.014586
0.439	0.000016	0.968	0.000858	0.762	0.000005
0.366	0.000001	0.763	0.001561	0.369	0.000008
0.149	0.000015	0.434	0.000500	0.358	0.000002
64.724	0.051151	57.836	0.095576	68.179	0.045744
75.804	0.018738	88.364	0.072064	79.024	0.018667
101.056	0.008112	108.081	0.097770	104.679	0.004225
124.749	0.063140	132.777	0.048594	127.024	0.071426
186.262	0.170631	182.072	0.034581	173.313	0.233345
201.138	0.107979	235.123	0.281319	197.689	0.048104
288.104	0.027262	283.266	0.361544	287.497	0.025851
305.066	0.144786	324.880	0.118141	303.998	0.139025
383.590	0.222522	383.803	0.062819	386.650	0.272662
426.658	0.486301	452.723	0.176074	419.079	1.050154
450.570	0.837510	463.067	0.752481	449.089	0.392016
460.925	0.898702	476.157	0.266374	456.134	1.384764
513.728	0.465591	534.949	0.688149	516.646	0.425666
537.939	1.457598	548.025	0.263491	534.126	1.386348
545.659	0.332765	568.084	0.304024	548.154	0.269426
573.210	0.222321	598.107	0.186374	575.564	0.218843
580.709	0.034636	614.050	2.185030	587.953	0.040561
619.992	0.167189	678.352	1.411235	620.274	0.132530
670.421	0.095824	712.757	1.440638	679.578	0.042298
677.616	1.795481	754.682	3.503697	693.730	2.440166
693.788	1.249265	764.391	0.144036	696.549	0.777673
705.109	0.745832	790.386	0.820871	721.771	0.419503
725.080	0.795783	813.789	0.132946	721.902	1.098863
834.220	0.150487	887.077	0.699532	856.980	0.139503
863.514	0.208164	921.017	0.378737	882.977	0.906728
875.936	1.941747	933.800	0.059190	905.793	0.504390
919.528	0.378790	957.237	0.211141	929.947	0.079612
921.802	0.068463	987.568	0.299335	930.475	0.442098
957.760	0.055054	1012.355	0.090307	961.859	0.044533
969.042	0.048536	1015.695	0.193425	976.057	0.085658
974.821	0.264035	1042.279	0.629992	979.557	0.297785
997.760	0.407620	1048.705	0.111699	1015.393	0.456909
1028.333	0.303476	1068.480	0.185507	1035.599	0.252604
1066.648	0.279772	1095.658	2.191432	1086.341	0.542417

1107.564	0.826620	1102.037	1.121182	1119.681	0.404583
1167.146	3.016834	1164.449	0.021914	1176.652	2.117295
1173.502	0.872508	1217.569	2.893554	1184.583	1.365624
1196.587	0.095676	1240.275	2.038476	1196.545	0.187806
1230.464	0.680610	1276.555	1.008369	1237.805	0.189937
1235.551	0.046040	1289.964	0.762183	1258.432	0.311129
1291.908	9.386658	1329.758	14.401108	1312.973	6.947077
1346.955	0.166528	1347.543	3.055715	1342.837	0.377881
1357.779	0.055921	1355.775	1.717345	1370.854	0.106276
1375.834	0.130592	1415.090	0.219322	1393.979	0.184996
1397.894	1.646785	1422.518	9.327067	1405.385	1.774642
1411.220	3.144756	1452.109	0.274952	1421.460	3.263078
1428.049	0.259835	1481.981	11.812656	1450.965	1.038732
1465.111	2.065266	1506.230	5.327646	1470.530	1.406968
1468.666	5.388622	1532.084	6.332039	1486.768	10.782498
1587.883	0.085386	1563.067	2.364381	1625.959	0.096370
1671.921	0.570420	1653.727	0.487097	1712.551	0.321241
1700.137	16.983379	1778.123	25.283326	1746.578	18.604195
1725.835	1.474223	1808.162	0.782850	1758.506	0.837411
2968.386	1.335271	3068.779	0.805295	3001.054	1.191478
3102.101	0.308980	3122.681	0.869469	3133.057	0.223444
3170.873	0.462182	3156.451	0.141625	3205.771	0.282217
3178.495	0.101209	3238.171	0.128499	3210.139	0.021196
3203.057	0.326464	3254.093	0.093904	3231.833	0.228948
3209.017	0.048382	3255.196	0.377561	3240.733	0.073145
3215.745	0.450197	3283.481	0.139115	3248.750	0.258939
3227.752	0.130239	3284.002	0.189309	3261.670	0.067244
3247.591	0.131714	3309.490	0.016857	3269.590	0.129475
3622.404	4.654350	3643.050	5.430093	3664.681	5.147766

D.8—**P(S_0)** PCM (methanol)

B3LYP		**M06HF**		**PBE0**	
FREQ (cm^{-1})	**IR ITENS.**	**FREQ (cm^{-1})**	**IR ITENS.**	**FREQ (cm^{-1})**	**IR ITENS.**
5.527	0.021581	12.516	0.037001	6.802	0.038992
4.393	0.038597	6.123	0.028488	4.774	0.022291
3.879	0.008484	4.244	0.010223	3.736	0.009427
0.473	0.000028	3.076	0.001738	0.489	0.000017
0.285	0.000016	2.160	0.000446	0.232	0.000010
0.093	0.000003	1.330	0.000408	0.243	0.000010
52.078	0.054174	51.259	0.065142	61.570	0.054720
81.088	0.051037	86.089	0.061393	83.169	0.052987
127.397	0.157917	139.386	0.168917	131.540	0.149090
140.757	0.043844	151.993	0.059920	147.470	0.042041
177.459	0.017687	177.733	0.033761	183.572	0.019311
286.936	0.145941	287.830	0.173113	290.123	0.127222
302.687	0.183370	303.485	0.173478	307.336	0.200881
392.656	0.131664	394.380	0.125683	396.411	0.110089
431.059	0.035941	438.403	0.049929	433.768	0.033320
446.702	1.613167	463.992	1.814998	454.058	1.605881
501.500	0.520591	513.353	0.622399	506.867	0.509749
529.825	0.549653	534.868	0.580408	535.904	0.534357
553.767	1.284325	558.366	1.965310	560.246	1.566270
563.514	0.348888	570.447	0.258082	567.835	0.248876
601.475	0.243135	614.753	0.118627	608.517	0.165243
627.555	0.031357	618.610	0.058139	625.177	0.040335
709.392	1.547510	722.618	1.067763	714.458	1.452889
710.199	1.064981	734.723	0.155068	717.022	1.585227
724.260	0.597894	746.401	2.591525	732.749	0.578207
750.573	0.282687	795.314	0.407353	766.046	0.231889
775.434	1.177665	805.719	2.239665	778.494	1.468346
842.780	0.039763	881.143	0.028003	846.448	0.033248
874.949	0.348857	892.658	0.494836	886.713	0.367625
919.763	0.097028	955.714	0.067430	922.070	0.114896

950.620	0.121553	972.158	0.199721	959.430	0.081999
982.892	0.094895	1001.604	0.001566	989.061	0.007202
984.257	0.020612	1023.129	0.084812	994.850	0.104662
1005.220	0.004312	1040.620	0.007517	1007.598	0.002046
1008.350	0.019750	1045.114	0.049301	1011.562	0.009441
1011.022	0.080963	1060.034	0.261930	1026.578	0.179575
1041.436	0.396821	1062.192	0.129235	1051.628	0.379273
1059.496	0.095841	1076.813	0.137864	1069.379	0.119052
1078.521	0.976338	1099.952	1.096758	1094.692	1.062095
1103.918	0.119673	1116.483	0.212933	1112.447	0.166381
1165.518	0.053428	1165.364	0.107790	1165.217	0.049400
1189.709	0.903679	1200.131	0.050003	1194.281	0.202505
1195.143	1.799575	1212.740	1.179213	1200.833	1.538787
1203.742	2.212015	1244.386	2.184048	1230.986	2.399625
1244.527	0.081382	1272.592	0.285258	1253.947	0.286284
1288.475	6.980249	1298.313	0.773963	1310.617	5.731255
1303.489	4.098798	1329.995	5.771795	1330.326	1.863955
1337.687	0.006355	1344.547	2.653360	1340.536	0.383403
1357.518	0.383368	1357.486	0.373936	1389.978	0.395956
1419.612	0.536710	1442.893	0.884943	1428.944	0.779848
1444.104	7.699238	1486.753	4.928225	1454.617	4.414157
1464.534	2.027447	1495.579	6.093724	1480.225	0.994563
1474.754	0.804070	1507.916	1.151179	1484.648	4.173221
1484.479	4.327329	1538.718	6.774572	1496.514	8.294923
1524.102	1.931954	1554.801	2.942038	1537.516	2.770597
1628.650	0.185781	1684.600	0.266363	1658.168	0.196141
1647.349	0.981026	1700.087	1.247080	1678.395	1.101403
1727.949	19.520657	1772.676	25.694005	1766.121	15.795408
1750.501	0.972421	1802.669	0.896636	1783.359	5.723326
2950.089	2.121651	3063.997	1.078997	2984.594	1.840452
3072.976	0.449999	3169.473	0.110698	3106.622	0.307264
3171.587	0.035243	3251.893	0.023520	3203.665	0.036414
3180.559	0.475591	3259.198	0.100160	3212.798	0.315575
3195.358	0.818016	3267.896	0.121386	3227.261	0.568582
3212.413	0.127492	3275.095	0.027127	3238.569	0.096462
3212.750	0.076312	3283.904	0.150348	3245.829	0.049387
3231.988	0.243303	3295.699	0.014374	3264.776	0.025134
3232.466	0.078925	3305.942	0.020283	3265.616	0.145269
3621.545	3.445880	3633.503	4.829957	3664.972	3.975004

D- Molecular Orbitals

E.1- S_0 PCM(methanol)

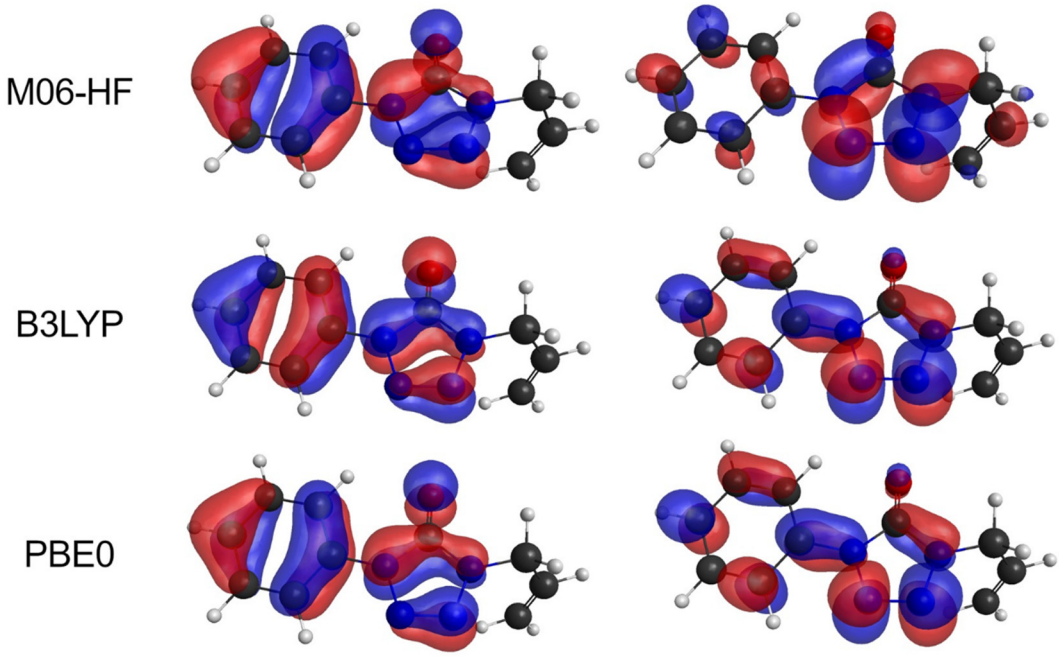


Figure S1. HOMO and LUMO of S0 (for M06-HF it is represented the LUMO+2 orbital instead of LUMO.

E.2- T_1 PCM(methanol)

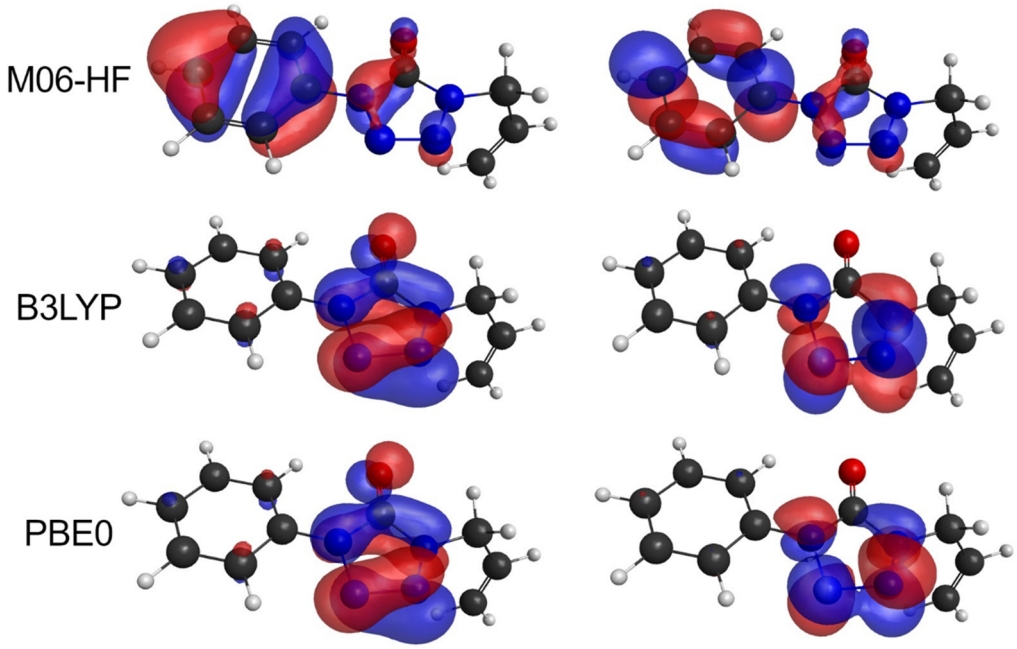


Figure S2. SOMO of T_1.

E.3- M1 PCM(methanol)

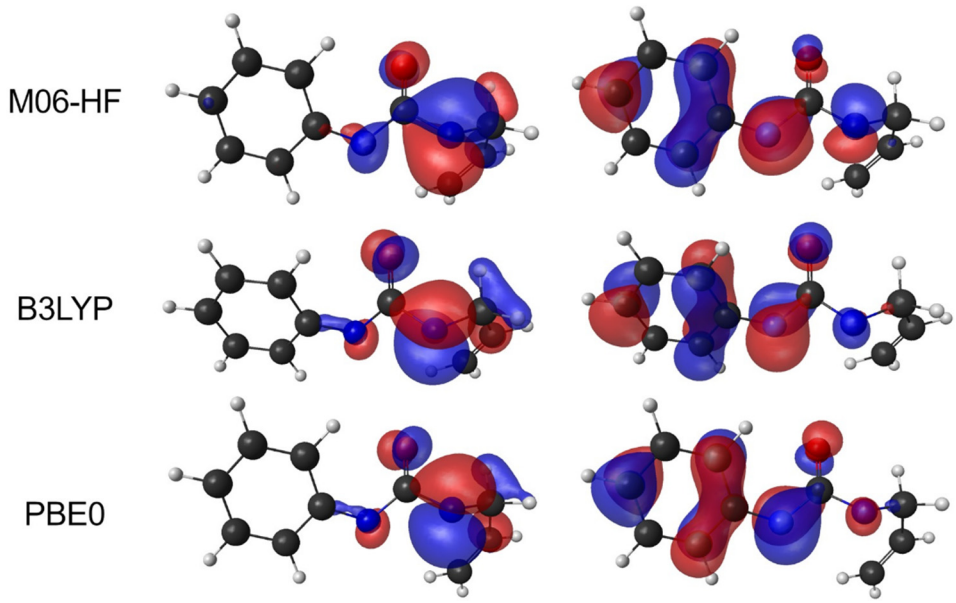


Figure S3. SOMO of M1.

E.4- M2 PCM(methanol)

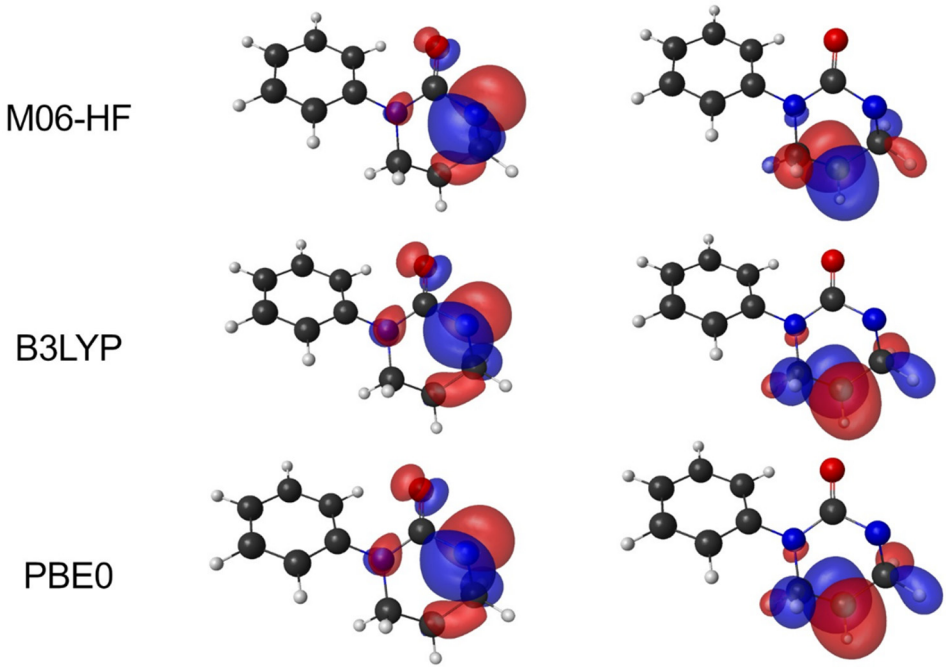


Figure S4. SOMO of M2.