

Table 1. The energies of tautomers(a.u) at DFT/6-311++G(d,p) level in different media and the relative energies compared to the most stable isomer 2TU1. The relative energies in brackets in kcal mol⁻¹ (in brackets Kcal/mole).

Isomers	$\Delta E(\text{gas})$	$\Delta E(\text{water})$	$\Delta E(\text{Acetonitrile})$
2TU1	-737.899473020 (0.0000)	-737.916336580(0.0000)	-737.915900370(0.0000)
2TU2	-737.88090388(11.6523)	-737.89353095(14.3107)	-737.89321425(14.2358)
2TU3	-737.87768488(13.6723)	-737.89233375(15.0620)	-737.89229300(14.8138)
2TU4	-737.87925325(12.6881)	-737.89911925(10.8040)	-737.86856173(29.7054)
2TU5	-737.86747854(20.0768)	-737.89378865(14.1490)	-737.89418033(13.6295)
2TU6	-737.88025401(12.0601)	-737.88803863(17.7572)	-737.88784348(17.6060)
2TU7	-737.87957496(12.4862)	-737.88785780(17.8707)	-737.88773617(17.6733)
2TU8	-737.87169145(17.4332)	-737.88478499(19.7989)	-737.88454688(19.6746)
2TU9	-737.86363640(22.4878)	-737.88764167(18.0063)	-737.88693953(18.1732)
2TU10	-737.85926764(25.2293)	-737.88308063(20.8684)	-737.88366617(20.2273)
2TU11	-737.86186485(23.5995)	-737.88792579(17.8280)	-737.88715114(18.0404)
2TU12	-737.86670631(20.5614)	-737.88899187(17.1591)	-737.88836509(17.2786)

Table 2. The zero dipole moments (μ) in Debye units, for the tautomers at DFT/6-311++G(d,p) level in different media.

Isomers	Gas	Water	Acetonitrile
2TU1	4.7462	6.6964	6.6414
2TU2	2.9654	4.1644	4.1331
2TU3	2.1055	2.8698	3.0960
2TU4	5.7112	9.0025	8.9053
2TU5	8.5147	12.0860	12.6761

2TU6	1.3385	1.9524	1.9356
2TU7	2.1036	2.8607	2.9737
2TU8	4.1486	5.5645	5.6054
2TU9	8.1244	12.6227	12.4880
2TU10	6.5580	9.5422	10.3299
2TU11	8.3876	12.3290	12.2103
2TU12	6.7169	9.9378	9.8397

Table 3. The enthalpy (ΔH), Gibbs free energy (ΔG) values in kcal/mol and entropy (ΔS) in kcal/mol Kelvin, for the tautomers at DFT/6-311++G(d,p) level in different media.

Isomers	Gas			Water			Acetonitrile		
	ΔH	ΔG	ΔS	ΔH	ΔG	ΔS	ΔH	ΔG	ΔS
2TU1 $\leftrightarrow$ 2TU2	9.3618	8.9859	0.00126	11.9327	11.5054	0.00143	11.8606	11.4357	0.0013
2TU1 $\leftrightarrow$ 2TU3	11.3435	10.5886	0.00253	12.6688	12.0865	0.00195	12.4611	11.8744	0.0025
2TU1 $\leftrightarrow$ 2TU4	12.4598	12.5471	-0.00029	10.5685	10.6438	-0.00025	10.6444	10.7210	-0.0003
2TU1 $\leftrightarrow$ 2TU5	19.5827	19.4214	0.00054	13.7230	13.5818	0.00047	13.3214	13.2907	0.0005
2TU1 $\leftrightarrow$ 2TU6	9.7885	9.7440	0.00015	15.2704	15.0182	0.00085	15.1249	14.8789	0.0001
2TU1 $\leftrightarrow$ 2TU7	10.1977	10.1236	0.00025	15.4204	15.1575	0.00088	15.1914	14.9404	0.0002
2TU1 $\leftrightarrow$ 2TU8	15.0006	14.8387	0.00054	17.2935	16.9290	0.00122	17.1567	16.8430	0.0005
2TU1 $\leftrightarrow$ 2TU9	21.8235	21.6641	0.00053	17.4843	17.3833	0.00034	17.6525	17.5571	0.0005
2TU1 $\leftrightarrow$ 2TU10	24.3863	23.9621	0.00142	20.2209	19.9636	0.00086	19.7929	19.7709	0.0014
2TU1 $\leftrightarrow$ 2TU11	21.0642	19.9109	0.00387	15.4876	14.7527	0.00246	15.6946	14.9410	0.0039
2TU1 $\leftrightarrow$ 2TU12	18.1168	17.3136	0.00269	14.8713	14.2871	0.00196	14.9868	14.3938	0.0027

Table 4. $\Delta\Delta H^0$ (solvent 1- solvent 2), and $T\Delta\Delta S^0$ (solvent 1- solvent 2), values in kcal/mole for the tautomers at DFT/6-311++G(d,p) level in different media.

Isomers	$\Delta\Delta H^0(G \rightarrow W)$	$T\Delta\Delta S^0(G \rightarrow W)$	$\Delta\Delta H^0(G \rightarrow A)$	$T\Delta\Delta S^0(G \rightarrow A)$	$\Delta\Delta H^0(A \rightarrow W)$	$T\Delta\Delta S^0(A \rightarrow W)$
2TU1 $\leftrightarrow$ 2TU2	-2.5709	-0.0506	-2.4988	-0.0119	-0.0721	-0.0387
2TU1 $\leftrightarrow$ 2TU3	-1.3253	0.1729	-1.1176	0.0089	-0.2077	0.1639
2TU1 $\leftrightarrow$ 2TU4	1.8913	-0.0119	1.8154	0.0029	0.0759	-0.0149
2TU1 $\leftrightarrow$ 2TU5	5.8597	0.0208	6.2613	0.0119	-0.4016	0.0089
2TU1 $\leftrightarrow$ 2TU6	-5.4819	-0.2087	-5.3364	0.0149	-0.1455	-0.2236
2TU1 $\leftrightarrow$ 2TU7	-5.2227	-0.1878	-4.9937	0.0149	-0.229	-0.2027
2TU1 $\leftrightarrow$ 2TU8	-2.2929	-0.2027	-2.1561	0.0119	-0.1368	-0.2146
2TU1 $\leftrightarrow$ 2TU9	4.3392	0.0566	4.1710	0.0089	0.1682	0.0477
2TU1 $\leftrightarrow$ 2TU10	4.1654	0.1669	4.5934	0.0059	-0.428	0.1610
2TU1 $\leftrightarrow$ 2TU11	5.5766	0.4203	5.3696	-0.0089	0.2070	0.4293
2TU1 $\leftrightarrow$ 2TU12	3.2455	0.2176	3.1300	-0.0029	0.1155	0.2206

Table 5. The equilibrium constants (K) and p^K_T values for the tautomers at DFT/6-311++G(d,p) level in different media.

Isomers	Gas		Water		Acetonitrile	
	K	p^K_T	K	p^K_T	K	p^K_T
2TU1 $\leftrightarrow$ 2TU2	2.58590 x10 ⁻⁷	6.5874	3.67804 x10 ⁻⁹	8.4344	4.13702 x10 ⁻⁹	8.3833
2TU1 $\leftrightarrow$ 2TU3	1.72864 x10 ⁻⁸	7.7623	1.37919 x10 ⁻⁹	8.8604	1.97305 x10 ⁻⁹	8.7049
2TU1 $\leftrightarrow$ 2TU4	6.33821 x10 ⁻¹⁰	9.1980	1.57485 x10 ⁻⁸	7.8028	1.38244 x10 ⁻⁸	7.8594
2TU1 $\leftrightarrow$ 2TU5	5.78831 x10 ⁻¹⁵	14.2374	1.10522 x10 ⁻¹⁰	9.9566	1.80669 x10 ⁻¹⁰	9.7431
2TU1 $\leftrightarrow$ 2TU6	7.19224 x10 ⁻⁸	7.1431	9.78253 x10 ⁻¹²	11.0095	1.23762 x10 ⁻¹¹	10.9074
2TU1 $\leftrightarrow$ 2TU7	3.78954 x10 ⁻⁸	7.4214	7.73274 x10 ⁻¹²	11.1117	1.11559 x10 ⁻¹¹	10.9525
2TU1 $\leftrightarrow$ 2TU8	1.32446 x10 ⁻¹¹	10.8780	3.88760 x10 ⁻¹³	12.4103	4.49510 x10 ⁻¹³	12.3473
2TU1 $\leftrightarrow$ 2TU9	1.31363 x10 ⁻¹⁶	15.8815	1.80569 x10 ⁻¹³	12.7434	1.34661 x10 ⁻¹³	12.8708
2TU1 $\leftrightarrow$ 2TU10	2.71552 x10 ⁻¹⁸	17.5661	2.31780 x10 ⁻¹⁵	14.6349	3.20855 x10 ⁻¹⁵	14.4937
2TU1 $\leftrightarrow$ 2TU11	2.53343 x10 ⁻¹⁵	14.5963	1.53138 x10 ⁻¹¹	10.8149	1.11441 x10 ⁻¹¹	10.9530
2TU1 $\leftrightarrow$ 2TU12	2.03113 x10 ⁻¹³	12.6923	3.36052 x10 ⁻¹¹	10.4736	2.80658 x10 ⁻¹¹	10.5518

Table 6. The inter conversion equilibrium constants (K) and p^K_T values for tautomers at DFT/6-311++G(d,p) level in different media.

Isomers	Gas		Water		Acetonitrile	
	K	p^K_T	K	p^K_T	K	p^K_T
2TU1 $\leftrightarrow$ 2TU2	2.5857 x10 ⁻⁷	6.5874	3.6781x10 ⁻⁹	8.4344	4.1370x10 ⁻⁹	8.3833
2TU2 $\leftrightarrow$ 2TU3	6.6853x10 ⁻²	1.1749	3.7500x10 ⁻¹	0.4259	4.7692 x10 ⁻¹	0.3215
2TU3 $\leftrightarrow$ 2TU4	3.6669x10 ⁻²	1.4357	1.1418x10 ¹	-1.0576	0.7006 x10 ⁻¹	-0.8455
2TU4 $\leftrightarrow$ 2TU5	9.13141x10 ⁻⁶	5.0395	7.0179x10 ⁻³	2.1538	1.3069x10 ⁻²	1.8838
2TU5 $\leftrightarrow$ 2TU6	1.2427x10 ⁷	-7.0944	8.8517x10 ⁻²	1.0530	6.8502x10 ⁻²	1.1643
2TU6 $\leftrightarrow$ 2TU7	5.2685x10 ⁻¹	0.2783	7.9045x10 ⁻¹	0.1021	9.0140x10 ⁻¹	0.0450
2TU7 $\leftrightarrow$ 2TU8	3.4950x10 ⁻⁴	3.4566	5.0278x10 ⁻²	1.2986	4.0293x10 ⁻²	1.3948
2TU8 $\leftrightarrow$ 2TU9	9.9178x10 ⁻⁶	5.0036	4.6446x10 ⁻¹	0.3330	2.9957x10 ⁻¹	0.5235
2TU9 $\leftrightarrow$ 2TU10	2.0674x10 ⁻²	1.6846	1.2836x10 ⁻²	1.8916	2.3827x10 ⁻²	1.6229
2TU10 $\leftrightarrow$ 2TU11	9.3295x10 ²	-2.9699	6.6064x10 ³	-3.8200	3.4732x10 ³	-3.5407
2TU11 $\leftrightarrow$ 2TU12	8.0168x10 ¹	-1.9040	0.2194x10 ⁻¹	-0.3413	0.2518 x10 ⁻¹	-0.4011
2TU1 $\leftrightarrow$ 2TU8	1.3244x10 ⁻¹¹	10.878	3.8879x10 ⁻¹³	12.4100	4.4951x10 ⁻¹³	12.347
2TU8 $\leftrightarrow$ 2TU9	9.9178x10 ⁻⁶	5.0036	4.6446x10 ⁻¹	0.3330	2.9957x10 ⁻¹	0.5235
2TU1 $\leftrightarrow$ 2TU7	3.7895x10 ⁻⁸	7.4214	7.7328x10 ⁻¹²	11.112	1.1156x10 ⁻¹¹	10.952
2TU8 $\leftrightarrow$ 2TU6	5.4308x10 ³	-3.7349	2.5162x10 ¹	-1.4007	2.7533x10 ¹	-1.4398
2TU2 $\leftrightarrow$ 2TU6	2.7816x10 ⁻¹	0.5557	2.6597x10 ⁻³	2.5752	2.9916x10 ⁻³	2.5241
2TU7 $\leftrightarrow$ 2TU3	4.5617x10 ⁻¹	0.3408	1.7837x10 ²	-2.2513	1.7686x10 ²	-2.2476
2TU3 $\leftrightarrow$ 2TU5	3.3483x10 ⁻⁷	6.4752	8.0128x10 ⁻²	1.0962	9.1569x10 ⁻²	1.0383
2TU6 $\leftrightarrow$ 2TU4	8.8128x10 ⁻³	2.0549	1.6098x10 ³	-3.2068	1.1170x10 ³	-3.0481
2TU6 $\leftrightarrow$ 2TU12	2.8238x10 ⁻⁶	5.5492	0.3434 x10 ⁻¹	-0.5359	0.2267 x10 ⁻¹	-0.3555
2TU11 $\leftrightarrow$ 2TU5	0.2284 x10 ⁻¹	-0.35881	0.7217x10 ⁻¹	-0.8583	1.6212x10 ¹	-1.2098
2TU7 $\leftrightarrow$ 2TU11	6.6857x10 ⁻⁸	7.1749	0.1980x10 ⁻¹	-0.2967	9.9894x10 ⁻¹	0.4600
2TU10 $\leftrightarrow$ 2TU6	2.6486x10 ¹⁰	-10.423	4.2206x10 ³	-3.6254	3.8572x10 ³	-3.5863
2TU8 $\leftrightarrow$ 2TU10	2.0504x10 ⁻⁷	6.6882	5.9617x10 ⁻³	2.2246	7.1379x10 ⁻³	2.1464

2TU9↔ 2TU7	2.8849×10^8	-8.4601	4.2823×10^1	-1.6317	8.2844×10^1	-1.9183
2TU1↔ 2TU9	1.3135×10^{-16}	15.882	1.8058×10^{-13}	12.743	1.3466×10^{-13}	12.871
2TU4↔ 2TU12	3.2043×10^{-4}	3.4943	2.1338×10^{-3}	2.6708	2.0302×10^{-3}	2.6925
2TU1↔ 2TU4	6.3387×10^{-10}	9.1980	1.5748×10^{-8}	7.8028	1.3824×10^{-8}	7.8594
2TU9↔ 2TU12	1.5463×10^3	-3.1893	1.8609×10^2	-2.2697	2.0842×10^2	-2.3189
2TU2↔ 2TU7	1.4655×10^{-1}	0.8340	2.1024×10^{-3}	2.6773	2.6966×10^{-3}	2.5692
2TU7↔ 2TU10	7.1662×10^{-11}	10.1450	2.9974×10^{-4}	3.5233	2.8761×10^{-4}	3.5412
2TU3↔ 2TU6	0.41608×10^{-1}	-0.6191	7.0927×10^{-3}	2.1492	6.2726×10^{-3}	2.2026
2TU6↔ 2TU11	3.5224×10^{-8}	7.4532	0.1565×10^{-1}	-0.1945	9.0045×10^{-1}	0.4554