

Table 1A. Cartesian coordinates of KET-KET stationary structure with total electronic energy of -1908.205675 (a.u.) evaluated at B3LYP/6-31G* level.

Atom	X (Å)	Y(Å)	Z(Å)
C	0.1697	-1.7661	-1.3942
H	0.5089	-0.8056	-1.7670
C	0.9659	-2.9040	-1.5265
H	1.9276	-2.8251	-2.0235
C	0.5172	-4.1184	-1.0117
H	1.1259	-5.0127	-1.1145
C	-0.7110	-4.1972	-0.3519
H	-1.0462	-5.1497	0.0508
C	-1.5359	-3.0773	-0.1854
C	-1.0510	-1.8835	-0.7411
S	-2.0303	-0.3186	-0.6132
O	-2.4947	-0.0429	0.8277
O	-1.2539	0.7901	-1.3707
N	-3.5148	-0.7530	-1.5575
H	-3.2125	-0.6346	-2.5293
C	-4.6670	0.1197	-1.2510
H	-5.5417	-0.4266	-1.6250
H	-4.7515	0.1503	-0.1605
C	-4.6121	1.5288	-1.8409
H	-5.5301	2.0766	-1.5997
H	-4.5203	1.4949	-2.9335
H	-3.7614	2.0924	-1.4469
C	-2.8483	-3.1992	0.5484
H	-2.9823	-4.2194	0.9185
H	-3.6873	-2.9530	-0.1107
H	-2.8935	-2.5075	1.3948
C	0.7966	0.7679	1.9427
H	0.0906	1.5057	1.5836
C	0.5091	-0.0046	3.0692
H	-0.4445	0.1202	3.5725
C	1.4482	-0.9255	3.5277
H	1.2409	-1.5223	4.4119
C	2.6611	-1.0868	2.8557
H	3.3885	-1.8070	3.2216
C	2.9731	-0.3477	1.7083
C	2.0076	0.5793	1.2865
S	2.3659	1.5640	-0.2470
O	3.5669	2.4977	-0.0091
O	2.4299	0.5793	-1.4423
N	0.9148	2.6066	-0.3687
H	0.1938	1.9997	-0.7840
C	1.1602	3.7947	-1.2114
H	2.0388	4.3044	-0.8086
H	1.3772	3.5221	-2.2542
C	-0.0741	4.6914	-1.1393
H	0.0809	5.5930	-1.7427
H	-0.2739	4.9914	-0.1060
H	-0.9599	4.1740	-1.5248
C	4.2792	-0.5648	0.9838

H	4.8344	0.3732	0.8817
H	4.8996	-1.2877	1.5208
H	4.1003	-0.9368	-0.0306

Table 2A. Cartesian coordinates of amide-amide structure (global minimum, Fig. 2a) with total electronic energy of -654.212088 (a.u.) evaluated at X3LYP/6-311G** level.

Atom	X (Å)	Y(Å)	Z(Å)
C	-3.0509	1.0896	-1.8884
C	-3.1536	0.6328	-0.4357
N	-1.8222	0.4104	0.1150
C	-1.4688	0.3832	1.4164
O	-0.3184	0.1048	1.7699
C	-2.5373	0.7204	2.4509
C	-2.0271	0.6148	3.8847
H	-1.0931	0.1181	-0.5465
H	-3.7544	-0.2852	-0.3791
H	-3.6752	1.3911	0.1531
H	-4.0466	1.2160	-2.3193
H	-2.5187	2.0410	-1.9566
H	-2.5047	0.3579	-2.4877
H	1.0444	-0.2989	0.5498
H	-3.3963	0.0577	2.2969
H	-2.9058	1.7330	2.2497
H	-2.8193	0.8714	4.5920
H	-1.6817	-0.3969	4.1022
H	-1.1832	1.2862	4.0477
N	1.7877	-0.5319	-0.1194
C	1.3934	-0.6633	-1.4025
O	0.2303	-0.4353	-1.7505
C	2.4384	-1.0963	-2.4252
H	3.2503	-0.3598	-2.4227
H	2.8912	-2.0353	-2.0874
C	1.8638	-1.2509	-3.8299
H	1.4298	-0.3129	-4.1780
H	2.6447	-1.5558	-4.5306
H	1.0706	-1.9997	-3.8465
C	3.0967	-0.8506	0.4381
H	3.8812	-0.5307	-0.2523
H	3.2089	-1.9354	0.5692
C	3.2778	-0.1506	1.7821
H	4.2406	-0.4174	2.2235
H	3.2395	0.9342	1.6603
H	2.4864	-0.4360	2.4786

Table 3A. Cartesian coordinates of amide-amide structure (global minimum, Fig. 2a) with total electronic energy of -654.315211 (a.u.) evaluated at B3LYP/6-31G* level.

Atom	X (Å)	Y(Å)	Z(Å)
C	-3.1253	0.4849	-1.9292
C	-3.1598	0.4913	-0.4006
N	-1.7988	0.4912	0.1255
C	-1.4189	0.5983	1.4191
O	-0.2307	0.4853	1.7618
C	-2.5078	0.8760	2.4528
C	-1.9516	1.0381	3.8668
H	-1.0347	0.3243	-0.5426
H	-3.7146	-0.3891	-0.0412
H	-3.7088	1.3751	-0.0484
H	-4.1422	0.4451	-2.3332
H	-2.6347	1.3859	-2.3118
H	-2.5682	-0.3802	-2.3033
H	1.1275	-0.1143	0.5579
H	-3.2425	0.0589	2.4155
H	-3.0584	1.7774	2.1497
H	-2.7595	1.2513	4.5755
H	-1.4338	0.1307	4.1902
H	-1.2269	1.8565	3.9078
N	1.8292	-0.4488	-0.1158
C	1.4496	-0.4135	-1.4136
O	0.3338	0.0072	-1.7580
C	2.4454	-0.9084	-2.4605
H	3.3660	-0.3127	-2.3786
H	2.7418	-1.9373	-2.2106
C	1.8859	-0.8454	-3.8828
H	1.5892	0.1742	-4.1440
H	2.6372	-1.1896	-4.6021
H	0.9955	-1.4736	-3.9805
C	3.0703	-1.0040	0.4134
H	3.9359	-0.5583	-0.0955
H	3.1197	-2.0869	0.2257
C	3.1610	-0.7419	1.9169
H	4.0733	-1.1879	2.3278
H	3.1727	0.3331	2.1256
H	2.3013	-1.1730	2.4420

Table 4A. Cartesian coordinates of amide-amide structure (local minimum, Fig. 2b) with total electronic energy of -654.311430 (a.u.) evaluated at B3LYP/6-31G* level.

Atom	X (Å)	Y(Å)	Z(Å)
C	-3.4817	-0.1033	-2.5751
C	-3.4817	-0.1045	-1.0357
C	-2.0685	-0.0986	-0.4583
O	-1.5407	0.9901	-0.1722
N	-1.4051	-1.2658	-0.2931
C	-1.8435	-2.6256	-0.5792
C	-0.8879	-3.3396	-1.5410
N	1.0847	1.1783	1.0565
C	1.7633	0.0157	1.1848
O	1.2793	-1.0604	0.7930
H	-0.4523	-1.1720	0.0882
H	-3.9506	0.8133	-0.6710
H	-4.0700	-0.9474	-0.6560
H	-2.8511	-2.6023	-1.0001
H	-1.9038	-3.1912	0.3616
H	-4.5048	-0.0280	-2.9604
H	-2.9114	0.7506	-2.9561
H	-3.0343	-1.0166	-2.9836
H	-1.2311	-4.3627	-1.7343
H	-0.8269	-2.8063	-2.4958
H	0.1207	-3.3917	-1.1171
H	0.1575	1.0894	0.6161
C	3.1617	0.0165	1.7958
H	3.2408	0.7245	2.6285
H	3.3016	-0.9887	2.2020
C	4.2530	0.3100	0.7492
H	4.1965	-0.4052	-0.0793
H	5.2516	0.2386	1.1964
H	4.1497	1.3179	0.3316
C	1.4871	2.5308	1.4202
H	2.4948	2.5117	1.8417
H	0.8196	2.9069	2.2086
C	1.4350	3.4787	0.2172
H	1.7295	4.4921	0.5139
H	2.1088	3.1380	-0.5765
H	0.4216	3.5245	-0.1959

Table 5A. Cartesian coordinates of ester-amide stationary structure with total electronic energy of -674.035569 (a.u.) evaluated at X3LYP/6-311G** level.

Atom	X (Å)	Y(Å)	Z(Å)
O	-1.5498	-1.3943	-1.0717
C	-1.0480	-0.7148	-0.2147
C	-1.7249	-0.3961	1.1059
O	0.1921	-0.2152	-0.4389
C	0.8565	0.6852	0.4815
C	-3.1242	-0.9974	1.2003
H	-1.0901	-0.7629	1.9202
H	-1.7599	0.6910	1.2345
C	2.2315	0.9758	-0.0824
H	0.2686	1.6029	0.5671
H	0.9173	0.2148	1.4666
H	-3.5832	-0.7502	2.1601
H	-3.7680	-0.6202	0.4046
H	-3.0928	-2.0833	1.1032
H	2.7565	1.6795	0.5697
H	2.8253	0.0609	-0.1443
H	2.1524	1.4129	-1.0791
O	1.5068	1.9382	-3.2681
C	0.9790	1.1559	-4.0515
C	0.9518	1.4457	-5.5531
C	1.6116	2.7772	-5.9015
N	0.4114	-0.0018	-3.6202
C	-0.3326	-0.9981	-4.3810
C	0.0835	-2.4180	-4.0016
H	0.4097	-0.1163	-2.6129
H	-0.1634	-0.8295	-5.4442
H	-0.4906	-3.1512	-4.5752
H	-0.1094	-2.5997	-2.9430
H	-0.0859	1.4335	-5.9041
H	1.4510	0.6256	-6.0821
H	1.5949	2.9436	-6.9819
H	1.0976	3.6093	-5.4182
H	2.6483	2.8029	-5.5642
H	-1.4076	-0.8757	-4.2024
H	1.1463	-2.5814	-4.1976

Table 6A. Cartesian coordinates of ester-amide stationary structure with total electronic energy of -674.378350 (a.u.) evaluated at B3LYP/6-31G* level

Atom	X (Å)	Y(Å)	Z(Å)
O	-1.3474	-1.6721	-0.9584
C	-0.8649	-0.7895	-0.2949
C	-1.6618	0.0601	0.6791
O	0.4641	-0.5463	-0.4196
C	1.1142	0.5886	0.2153
C	-3.1447	-0.3032	0.6940
H	-1.2238	-0.0569	1.6768
H	-1.5202	1.1138	0.4162
C	2.6037	0.4389	-0.0125
H	0.7488	1.5028	-0.2547
H	0.8782	0.5908	1.2826
H	-3.6819	0.3254	1.4079
H	-3.5896	-0.1650	-0.2926
H	-3.2881	-1.3479	0.9732
H	3.1330	1.2536	0.4890
H	2.9669	-0.5102	0.3879
H	2.8261	0.4942	-1.0782
O	1.0514	1.7634	-2.8084
C	0.7395	1.0185	-3.7335
C	0.5297	1.5490	-5.1502
C	0.7493	3.0561	-5.2529
N	0.5823	-0.3205	-3.5471
C	0.0362	-1.2915	-4.4923
C	0.3085	-2.7118	-4.0042
H	0.6395	-0.6127	-2.5769
H	0.4936	-1.1400	-5.4737
H	-0.1149	-3.4395	-4.7005
H	-0.1452	-2.8696	-3.0232
H	-0.4824	1.2832	-5.4775
H	1.2074	1.0146	-5.8261
H	0.5913	3.3974	-6.2791
H	0.0635	3.5955	-4.5976
H	1.7625	3.3235	-4.9488
H	-1.0460	-1.1486	-4.6132
H	1.3833	-2.8952	-3.9260

Table 7A. Cartesian coordinates of KET-amide structure (global minimum, Fig. 3a) with total electronic energy of -1281.111285 (a.u.) evaluated at X3LYP/6-311G** level.

Atom	X (Å)	Y(Å)	Z(Å)
C	3.8670	0.6570	-3.0131
C	2.7303	0.2756	-3.7201
C	1.4526	0.3428	-3.1591
C	1.3662	0.8048	-1.8329
C	2.4961	1.1883	-1.1141
C	3.7527	1.1155	-1.7062
C	0.2573	-0.0775	-3.9726
S	-0.2277	1.0115	-1.0132
O	0.0705	1.4770	0.3534
O	-1.0952	1.8210	-1.8647
N	-0.8536	-0.5304	-0.9435
C	-2.2799	-0.7292	-1.2736
C	-2.5521	-2.2201	-1.4332
O	-0.7831	-1.7147	1.6874
C	-0.9174	-1.1423	2.7727
C	-1.3847	-1.9047	4.0074
C	-1.7549	-3.3549	3.7126
N	-0.6453	0.1728	2.9231
C	-0.8701	0.9808	4.1185
C	-0.2255	2.3540	3.9648
H	2.3791	1.5440	-0.0989
H	4.6312	1.4186	-1.1477
H	4.8407	0.5975	-3.4882
H	2.8301	-0.0821	-4.7401
H	-0.6110	-0.9713	-0.0475
H	-2.9262	-0.3081	-0.4954
H	-2.4951	-0.1890	-2.1943
H	-3.6066	-2.3870	-1.6687
H	-1.9491	-2.6445	-2.2390
H	-2.3207	-2.7605	-0.5130
H	-0.4644	0.7350	-4.0692
H	0.5663	-0.3879	-4.9715
H	-0.2594	-0.9138	-3.4968
H	-0.3698	0.6608	2.0729
H	-0.4522	0.4729	4.9927
H	-0.4163	2.9616	4.8522
H	-0.6257	2.8853	3.0981
H	-2.2333	-1.3747	4.4548
H	-0.5877	-1.8602	4.7592
H	-2.0613	-3.8640	4.6299
H	-2.5783	-3.4157	2.9987
H	-0.9127	-3.8969	3.2810
H	-1.9451	1.0996	4.3045
H	0.8559	2.2692	3.8363

Table 8A. Cartesian coordinates of KET-amide structure (global minimum, Fig. 3a) with total electronic energy of -1281.531208 (a.u.) evaluated at B3LYP/6-31G*level.

Atom	X (Å)	Y(Å)	Z(Å)
C	3.8555	0.4692	-2.4881
C	2.8280	0.1233	-3.3623
C	1.4806	0.2741	-3.0205
C	1.2090	0.7905	-1.7389
C	2.2283	1.1445	-0.8563
C	3.5586	0.9828	-1.2305
C	0.4093	-0.1159	-4.0058
S	-0.4826	1.0824	-1.1810
O	-0.3814	1.6568	0.1759
O	-1.2183	1.8289	-2.1994
N	-1.1197	-0.4606	-1.1126
C	-2.5680	-0.6120	-1.3747
C	-2.9054	-2.0975	-1.4470
O	-0.8266	-1.6456	1.5219
C	-0.8464	-1.1017	2.6306
C	-1.0371	-1.9239	3.9017
C	-1.2641	-3.4075	3.6240
N	-0.6855	0.2339	2.7691
C	-0.7912	1.0169	3.9976
C	-0.0936	2.3643	3.8321
H	1.9682	1.5468	0.1141
H	4.3515	1.2579	-0.5434
H	4.8884	0.3375	-2.7944
H	3.0728	-0.2750	-4.3421
H	-0.8530	-0.9053	-0.2241
H	-3.1661	-0.1270	-0.5934
H	-2.7941	-0.1112	-2.3157
H	-3.9747	-2.2315	-1.6323
H	-2.3524	-2.5859	-2.2528
H	-2.6570	-2.6010	-0.5098
H	-0.2304	0.7327	-4.2536
H	0.8558	-0.4973	-4.9254
H	-0.2369	-0.8910	-3.5869
H	-0.6042	0.7533	1.8965
H	-0.3352	0.4647	4.8227
H	-0.2014	2.9628	4.7398
H	-0.5198	2.9316	3.0011
H	-1.8742	-1.5067	4.4736
H	-0.1544	-1.7876	4.5382
H	-1.3681	-3.9598	4.5616
H	-2.1677	-3.5659	3.0328
H	-0.4323	-3.8345	3.0623
H	-1.8450	1.1750	4.2637
H	0.9728	2.2300	3.6349

Table 9A. Cartesian coordinates of KET-ester structure (global minimum) with total electronic energy of -1300.965515 (a.u.) evaluated at X3LYP/6-311G** level

Atom	X (Å)	Y(Å)	Z(Å)
C	4.6712	1.2188	2.8203
C	5.0151	1.1058	1.4782
C	4.0281	0.9017	0.5189
C	2.6752	0.8030	0.8564
C	2.3559	0.9160	2.2220
C	3.3348	1.1234	3.1914
C	1.6485	0.5829	-0.2226
S	0.6474	0.8887	2.8002
N	0.1463	-0.6610	2.3931
C	-1.2964	-0.8460	2.1115
C	-1.5343	-2.2891	1.6819
O	0.6912	1.0543	4.2603
O	-0.1501	1.8189	2.0048
O	-0.0657	-2.1636	4.9264
C	0.3731	-1.5075	5.8421
C	-0.4983	-0.7737	6.8380
O	1.7117	-1.4369	5.9862
C	2.3306	-0.5390	6.9299
H	3.0331	1.2199	4.2253
H	5.4326	1.3860	3.5725
H	6.0524	1.1802	1.1725
H	4.3074	0.8210	-0.5258
H	0.4504	-1.3101	3.1221
H	-1.9054	-0.6152	2.9929
H	-1.5726	-0.1469	1.3226
H	-2.5949	-2.4446	1.4677
H	-0.9614	-2.5311	0.7840
H	-1.2430	-2.9804	2.4758
H	0.9145	1.3901	-0.2357
H	2.1309	0.5258	-1.1988
H	1.1013	-0.3456	-0.0448
C	-1.9884	-0.9993	6.6046
H	-0.2129	-1.0812	7.8499
H	-0.2544	0.2904	6.7580
C	3.8270	-0.7571	6.8355
H	2.0604	0.4874	6.6699
H	1.9731	-0.7539	7.9409
H	-2.5719	-0.4678	7.3594
H	-2.2868	-0.6332	5.6217
H	-2.2399	-2.0597	6.6545
H	4.3464	-0.0845	7.5225
H	4.0841	-1.7854	7.0964
H	4.1807	-0.5624	5.8216

Table 10A. Cartesian coordinates of KET-ester structure (global minimum) with total electronic energy of -1301.122905 (a.u.) evaluated at B3LYP/6-31G*level.

Atom	X (Å)	Y(Å)	Z(Å)
C	4.7025	1.2423	2.8212
C	5.0557	1.1158	1.4781
C	4.0738	0.9144	0.5074
C	2.7123	0.8286	0.8336
C	2.4024	0.9508	2.1953
C	3.3580	1.1588	3.1822
C	1.6828	0.6108	-0.2467
S	0.6453	0.8982	2.7879
N	0.1535	-0.7739	2.3393
C	-1.3072	-0.8943	2.1372
C	-1.6023	-2.3207	1.6761
O	0.6816	1.0682	4.3273
O	-0.2217	1.8605	1.9600
O	-0.0776	-2.1764	4.9431
C	0.3675	-1.5104	5.8598
C	-0.5063	-0.7669	6.8520
O	1.7086	-1.4501	6.0042
C	2.3310	-0.5430	6.9340
H	3.0339	1.2595	4.2117
H	5.4609	1.4071	3.5808
H	6.0989	1.1781	1.1804
H	4.3613	0.8224	-0.5367
H	0.4194	-1.3421	3.1558
H	-1.8696	-0.6722	3.0540
H	-1.5973	-0.1649	1.3773
H	-2.6747	-2.4331	1.4804
H	-1.0535	-2.5560	0.7585
H	-1.3196	-3.0448	2.4472
H	0.9299	1.4043	-0.2377
H	2.1616	0.5834	-1.2296
H	1.1532	-0.3344	-0.0860
C	-1.9973	-0.9983	6.6116
H	-0.2241	-1.0671	7.8702
H	-0.2663	0.3001	6.7654
C	3.8312	-0.7578	6.8287
H	2.0561	0.4831	6.6679
H	1.9814	-0.7479	7.9528
H	-2.5881	-0.4630	7.3621
H	-2.2896	-0.6361	5.6223
H	-2.2473	-2.0619	6.6651
H	4.3555	-0.0799	7.5112
H	4.0946	-1.7874	7.0904
H	4.1768	-0.5646	5.8084