

Supporting Information for :

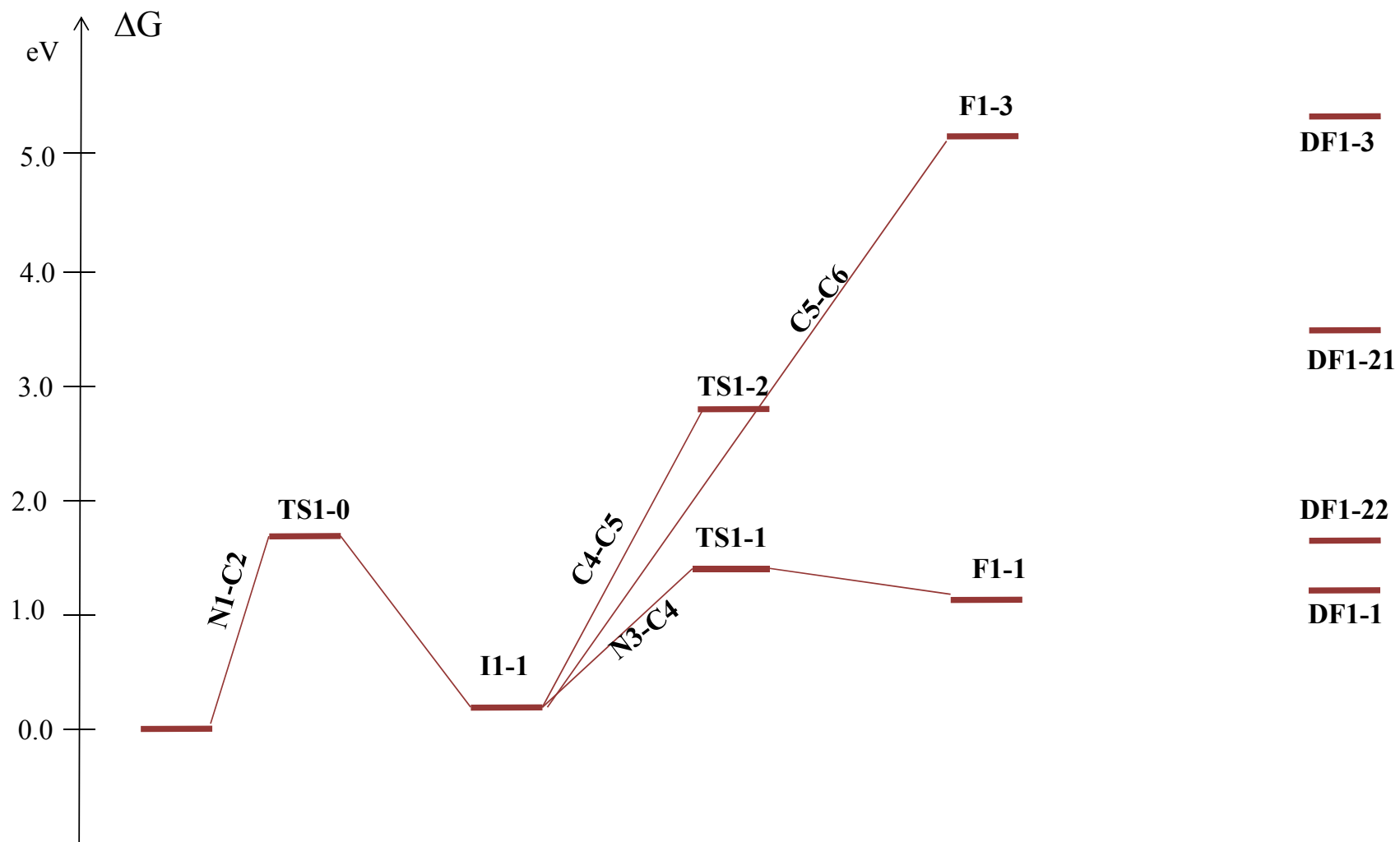
DFT study of the Fragmentation Mechanism of Uracil RNA bases

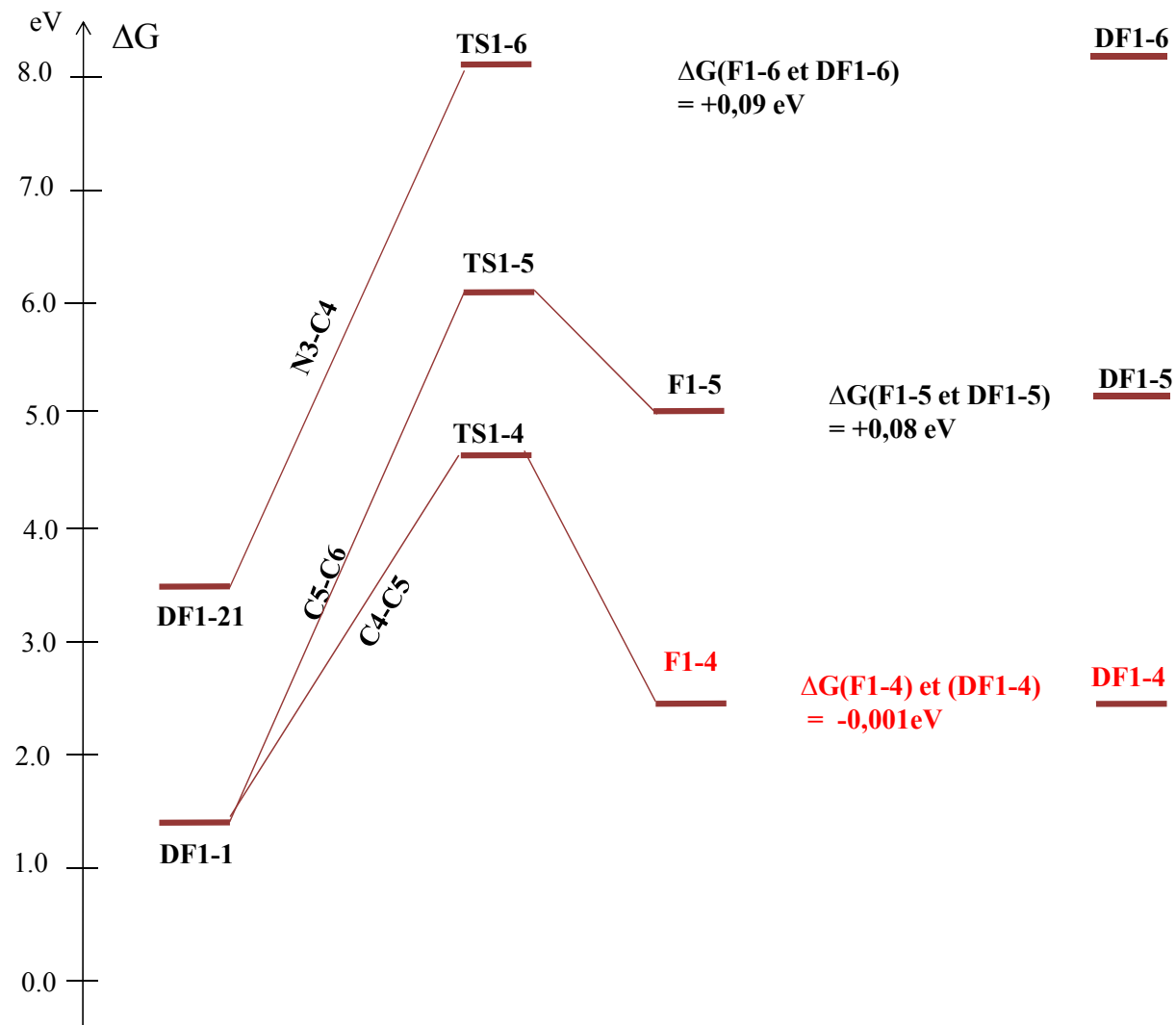
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Henry CHERMETTE¹,

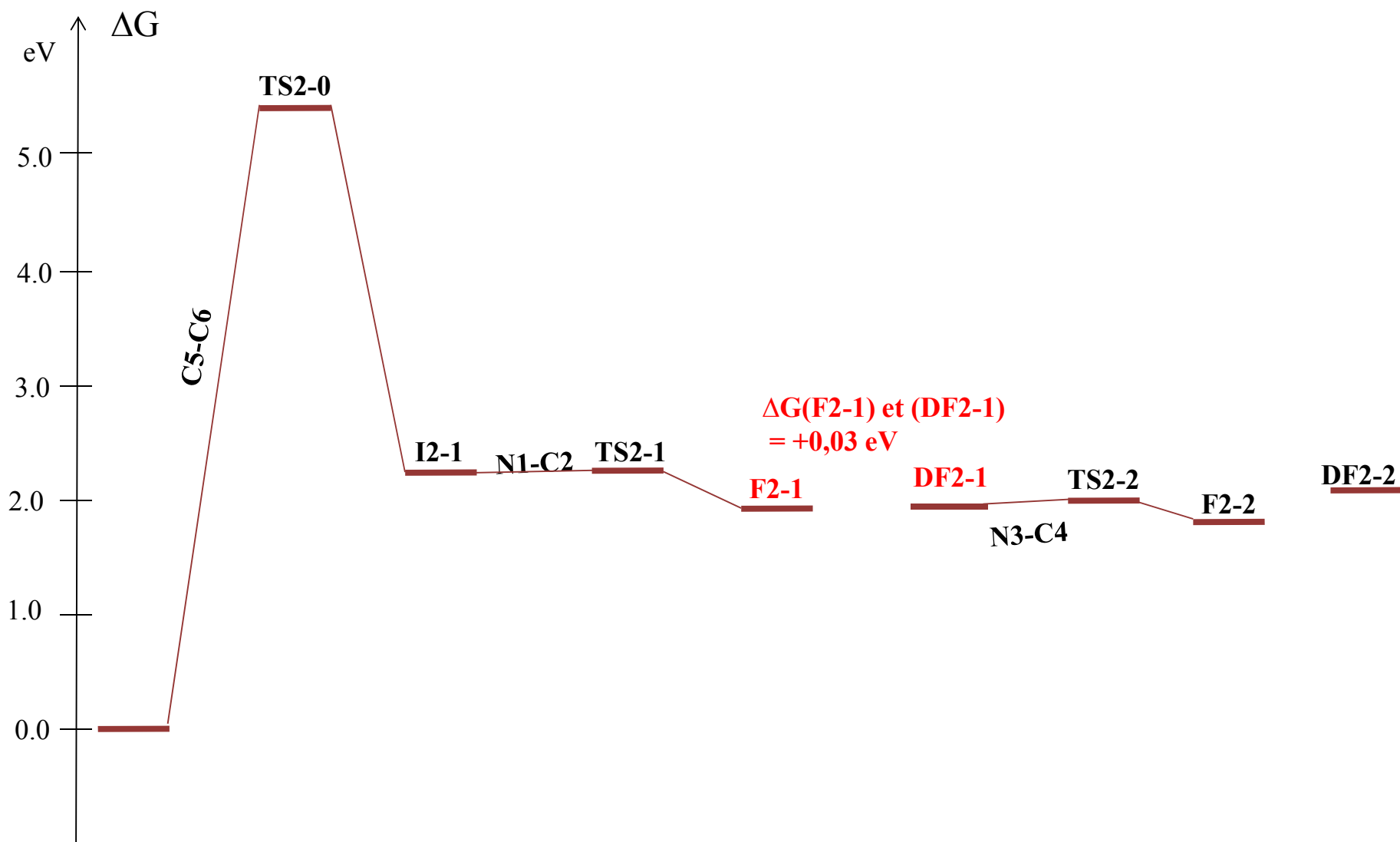
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5280; 43 Bd du 11 novembre 1918; 69622 Villeurbanne, Cedex, FRANCE

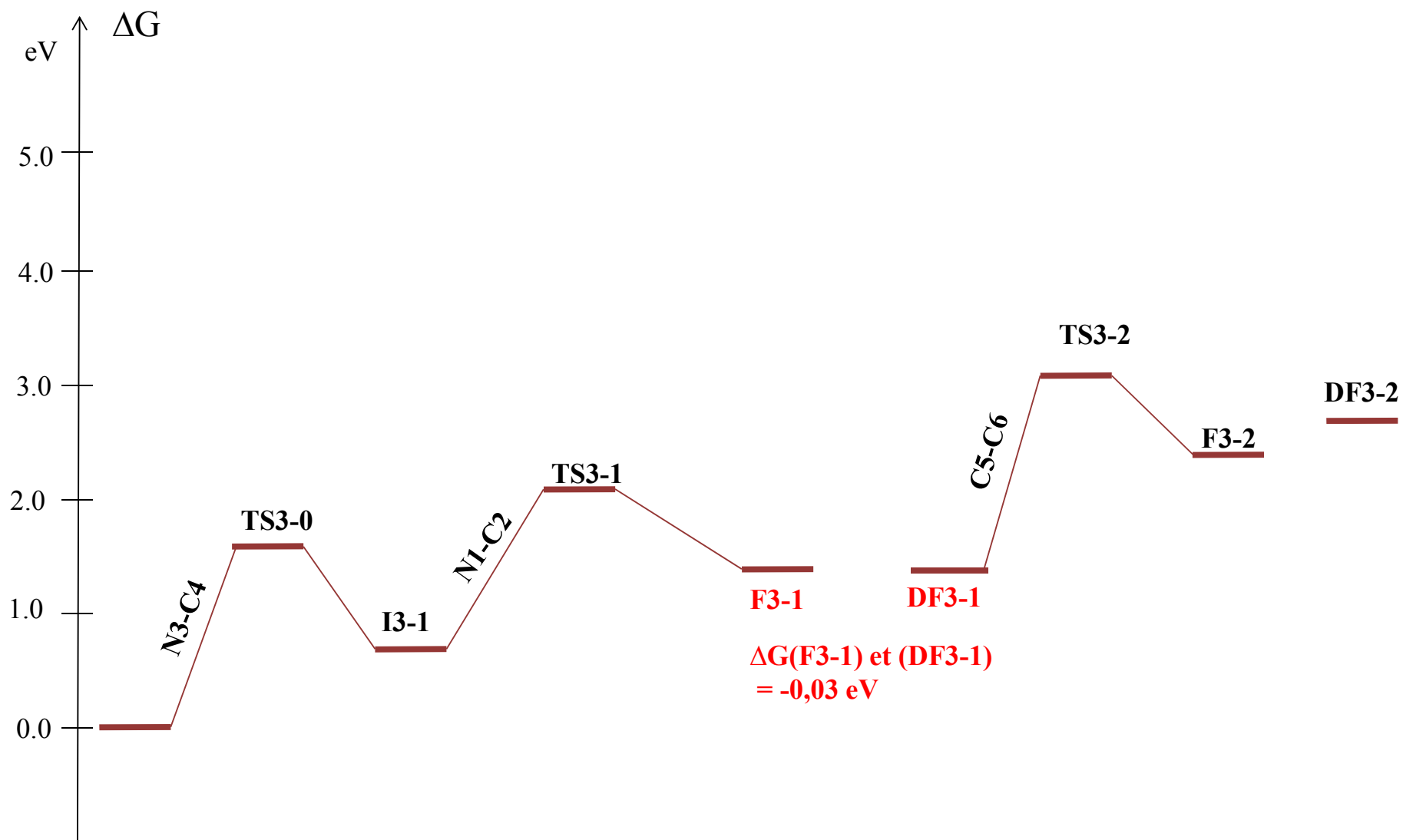
² Université de Lyon; Université Claude Bernard-Lyon1; Institut de Physique Nucléaire de Lyon,
CNRS/IN2P3 UMR 5822, 43 Bd du 11 novembre 1918, 69622 Villeurbanne Cedex, FRANCE

Free energy diagrams :









Cartesian Coordinates :

Points of figure 3:

➤ U+ :

	X	Y	Z
C	-0.000449	0.031297	-0.000001
N	0.069143	1.404488	-0.000006
C	1.234373	2.196311	-0.000004
C	2.492120	1.434006	0.000005
C	2.474722	0.028920	0.000010
N	1.306713	-0.604512	0.000008
H	-0.829157	1.897679	-0.000012
H	3.428133	1.992715	0.000007
H	3.385594	-0.574665	0.000017
O	1.202480	3.420282	-0.000009
O	-0.992789	-0.661847	-0.000002
H	1.258068	-1.630641	0.000011

➤ TS1-0

C	-0.424159	0.340162	0.764681
N	-0.076626	1.122235	-0.160210
C	1.286384	2.089587	-0.016236
C	2.510365	1.456531	-0.418259
C	2.786525	0.086065	-0.716873
N	1.876600	-0.848653	-0.637563
H	-0.355718	0.889779	-1.119702
H	3.336044	2.172359	-0.454497
H	3.830270	-0.115768	-0.999863
O	1.055386	3.190639	0.362448
O	-0.716911	-0.288936	1.683988
H	2.282912	-1.767557	-0.868050

➤ I1-1

C	-0.929799	0.846663	0.870423
N	0.162173	0.845358	0.262402
C	1.190794	1.775920	0.477615
C	2.423855	1.588060	-0.299351
C	2.872564	0.394963	-0.912168
N	2.152523	-0.701861	-1.022940
H	1.189113	-0.718205	-0.662420
H	3.099144	2.444032	-0.294256
H	3.873256	0.371723	-1.351537
O	1.171687	2.677099	1.311227

O	-1.967601	0.735690	1.370656
H	2.524552	-1.532465	-1.485239

➤ TS1-1

C	-1.125358	0.928631	0.325186
N	-0.011020	0.407046	0.384269
C	1.826895	1.573954	1.141370
C	2.425116	1.579155	-0.100727
C	2.696654	0.482419	-0.940667
N	2.235660	-0.741089	-0.833077
H	1.462300	-0.941966	-0.189304
H	2.846925	2.555031	-0.363743
H	3.390255	0.671513	-1.763582
O	1.610785	1.799566	2.249881
O	-2.206686	1.406556	0.266840
H	2.513633	-1.455736	-1.503086

➤ F1-1

C	-1.779445	0.172663	0.600275
N	-0.598574	0.275638	0.269213
C	2.202280	2.239165	0.734265
C	3.181691	1.658787	0.003881
C	3.045068	0.498475	-0.780737
N	1.974996	-0.239710	-0.961180
H	1.054442	-0.048922	-0.523521
H	4.148977	2.166109	0.049361
H	3.946621	0.172880	-1.304348
O	1.395567	2.759685	1.368598
O	-2.915599	0.081390	0.923227
H	2.035923	-1.058733	-1.562113

➤ DF1-1 :

DF1-1b[•] :

C	-1.197074	0.842177	0.385701
N	-0.050484	0.390001	0.417667
O	-2.307683	1.280164	0.354738

DF1-1a⁺ :

C	1.921218	1.661654	1.059382
C	2.657184	1.620383	-0.076811
C	2.743824	0.517332	-0.939447
N	2.155485	-0.655792	-0.831072
H	1.535345	-0.908549	-0.062146
H	3.211298	2.534659	-0.306371

H	3.381557	0.642719	-1.817486
O	1.301721	1.712216	2.026882
H	2.312767	-1.371886	-1.537676

➤ TS1-2 :

C	0.428840	0.871688	2.372116
N	0.873027	1.401474	1.336547
C	1.839434	2.206217	1.042570
C	2.356115	1.437233	-1.528288
C	2.258234	0.093172	-1.733089
N	1.129771	-0.635178	-1.718506
H	0.220913	-0.178675	-1.731946
H	3.122468	2.139566	-1.850366
H	3.181425	-0.490367	-1.874135
O	2.549553	3.106356	1.248727
O	-0.068880	0.275891	3.227077
H	1.158123	-1.629633	-1.920597

➤ DF1-22 :

DF1-2a[•] :

C	-0.903679	0.962834	1.599267
N	-0.297496	1.746307	0.873521
C	0.829611	2.536866	1.018124
O	1.322087	3.291005	0.235765
O	-1.572190	0.198837	2.193354

DF1-1b⁺:

C	3.520293	0.822025	-0.447486
C	2.846419	-0.029506	-1.138492
N	2.184279	-0.864372	-1.815258
H	1.157031	-0.825117	-1.860929
H	3.866073	1.755146	-0.906698
H	3.754962	0.618226	0.603847
H	2.648503	-1.614135	-2.345348

➤ DF1-21

DF1-2a⁺ :

C	-0.885491	0.946971	1.605106
N	0.030456	1.444304	0.911946
C	0.654048	2.514966	0.734920

O	1.286277	3.437494	0.490363
O	-1.706957	0.392114	2.177696

DF1-2b[•]:

C	3.057347	1.323623	-0.893727
C	3.112557	0.002055	-0.899513
N	2.151908	-0.896363	-1.390130
H	1.497944	-0.469667	-2.044651
H	3.639897	2.146167	-0.495579
H	3.966002	-0.494683	-0.409790
H	2.551905	-1.748865	-1.776973

➤ F1-3

C	-0.411744	0.927015	0.849073
N	0.616088	1.138473	0.167830
C	1.024117	2.481660	-0.237322
C	2.199921	2.534485	-1.027790
C	2.996744	-1.471730	0.179158
N	2.236007	-0.864635	-0.604740
H	1.547731	-0.056241	-0.260406
H	2.696186	3.410427	-1.447023
H	3.740928	-2.266380	0.049667
O	0.397455	3.485696	0.080776
O	-1.341220	0.632004	1.474495
H	2.210445	-1.077485	-1.619841

➤ DF1-3

DF1-3b^{••}:

C	-0.432074	0.920715	0.862832
N	0.531403	1.274899	0.194044
C	1.005744	2.530678	-0.236192
C	2.195533	2.492866	-1.019028
H	2.729012	3.341416	-1.450612
O	0.457283	3.611545	0.025620
O	-1.306098	0.437640	1.483375

DF1-3a^{•+}:

C	2.991610	-1.458288	0.186265
N	2.226873	-0.851445	-0.605529
H	1.590865	-0.108690	-0.271084
H	3.730386	-2.259154	0.055982

H 2.192120 -1.058894 -1.621796

Points of figure 4 :

➤ TS1-4

C	1.974645	0.156330	2.025942
C	2.363604	1.998074	-0.513472
C	2.487594	0.837163	-1.044019
N	2.411151	-0.471458	-1.073646
H	2.333800	-0.944888	-0.169119
H	2.888489	2.925477	-0.293952
H	2.514901	1.503327	-2.014210
O	1.705533	0.262333	3.122842
H	2.379064	-1.001021	-1.939695

➤ F1-4

C	0.767361	-0.486783	1.848875
C	3.402940	1.980619	-1.316662
C	2.910547	0.836840	-0.985906
N	2.418091	-0.268883	-0.639580
H	1.831854	-0.363681	0.237011
H	4.394611	2.278270	-0.960893
H	2.835176	2.660022	-1.960688
O	0.146207	-0.541165	2.794870
H	2.573850	-1.113475	-1.205234

➤ DF1-4 :

DF1-4a+ :

C	0.767361	-0.486783	1.848875
C	3.402940	1.980619	-1.316662
C	2.910547	0.836840	-0.985906
N	2.418091	-0.268883	-0.639580
H	1.831854	-0.363681	0.237011
H	4.394611	2.278270	-0.960893
H	2.835176	2.660022	-1.960688
O	0.146207	-0.541165	2.794870
H	2.573850	-1.113475	-1.205234

DF1-4b :

C	0.000000	0.000000	1.581248
O	0.000000	0.000000	2.721842

➤ TS1-5

C	2.376517	1.136969	0.986140
C	2.638107	2.383022	0.725752
C	2.551798	0.401595	-1.535787
N	2.089936	-0.655282	-1.087460
H	1.879342	-0.669308	-0.000792
H	3.499252	3.040734	0.665120
H	2.867525	0.763338	-2.519254
O	1.901089	0.077719	1.314778
H	1.886809	-1.515494	-1.622997

➤ F1-5

C	2.560072	1.924363	0.529971
C	3.138376	2.852335	0.023537
C	2.175967	-0.983151	-1.087467
N	2.313328	-1.711042	-1.960648
H	1.277886	1.019080	1.639786
H	3.627433	3.715975	-0.382269
H	2.012956	-0.290016	-0.196560
O	1.993466	0.810301	1.000389
H	2.443957	-2.342236	-2.749909

➤ DF1-5

DF1-5a⁺ :

C	2.18541360	-0.90202201	-0.98333370
N	2.36088700	-1.67833900	-1.93419700
H	2.01884108	-0.31512470	-0.20365098
H	2.74849543	-1.73498942	-2.87476986

DF1-5b :

C	2.543151	1.881414	0.524643
C	3.102401	2.797807	-0.032657
H	1.225112	1.093121	1.617598
H	3.617477	3.629714	-0.462618
O	1.970817	0.815736	1.049739

Points of figure 4 :

➤ TS1-6

C	-0.295844	-0.289008	1.532488
N	0.408301	0.648975	1.038572
C	0.149220	4.461059	0.877895
O	0.199722	5.586622	0.759040
O	-0.934123	-1.158583	1.982157

➤ DF1-6

DF1-6a⁺ :

C	-1.163957	-0.375052	0.000000
N	-0.532516	0.786931	0.000000
O	-1.705620	-1.390733	0.000000

DF1-6b :

C	0.000000	0.000000	1.581248
O	0.000000	0.000000	2.721842

Les points de figure 5 :

➤ TS2-0

C	0.034372	0.500376	0.548710
N	0.149482	1.356766	-0.502516
C	1.285829	1.664459	-1.306207
C	2.481896	0.903558	-1.229995
C	1.905152	0.161684	2.123193
N	1.431715	-0.051767	0.985646
H	-0.722463	1.801345	-0.800446
H	3.417423	1.043683	-1.780436
H	2.862248	-0.108591	2.583756
O	1.234625	2.588597	-2.116497
O	-0.928416	0.154508	1.164060
H	1.947340	-0.606513	0.222208

➤ I2-1

C	-0.161406	0.101088	0.174814
N	0.011065	1.393170	-0.026456
C	1.250859	2.249797	-0.041284
C	2.307213	1.837404	-0.905939
C	2.114007	-1.445980	0.735749
N	1.423764	-0.598006	0.365354
H	-0.850598	1.940379	0.079385
H	3.233989	2.408880	-0.865663
H	2.796274	-2.219784	1.067258
O	1.198218	3.277517	0.613938
O	-1.009019	-0.709697	0.285984
H	2.184970	1.045892	-1.644434

➤ TS2-1

C	-0.151076	0.143611	0.213105
N	0.092782	1.406456	-0.051477
C	1.373267	2.238977	-0.059508
C	2.318730	1.925183	-1.075873
C	2.025841	-1.548093	0.934422
N	1.437411	-0.656966	0.493193
H	-0.749610	1.989478	0.014773
H	3.237298	2.510650	-1.098522
H	2.617182	-2.364340	1.330668
O	1.407047	3.172017	0.722315
O	-1.020847	-0.635561	0.348654
H	2.132811	1.159663	-1.828566

➤ F2-1

C	-0.583079	0.410335	-0.325719
N	-0.193287	1.595004	-0.138428
C	1.391078	2.154448	-0.204723
C	2.183569	1.414350	-1.110605
C	2.497821	-1.339604	1.568198
N	1.867566	-0.638568	0.895959
H	-0.826799	2.264609	0.311677
H	3.230498	1.704539	-1.188829
H	3.078833	-1.993921	2.199972
O	1.564510	3.101221	0.493598
O	-0.889016	-0.673898	-0.567457
H	1.780559	0.609700	-1.720645

➤ DF2-1

DF2-1a^{•+}:

C	-0.338968	0.390198	-0.337283
N	-0.119260	1.573391	0.038805
C	1.319703	2.496796	-0.121146
C	2.328907	1.790247	-0.817921
H	-0.860088	2.105283	0.511560
H	3.278690	2.307771	-0.959188
O	1.211915	3.567309	0.377830
O	-0.427666	-0.693900	-0.723491
H	2.183442	0.783141	-1.207009

DF2-1b:

C	2.133008	-1.546912	0.000000
N	1.485058	-0.585184	0.000000
H	2.737682	-2.437620	0.000000

➤ TS2-2

C	-0.605455	0.594625	-0.892871
N	-0.236730	1.766199	-0.704879
C	1.681934	2.511049	0.230691
C	2.554632	1.860152	-0.628115
H	-0.858961	2.544052	-0.941568
H	3.471666	2.398658	-0.891673
O	1.320286	3.223763	1.060163
O	-0.812753	-0.542659	-1.018423
H	2.345828	0.859667	-1.002328

➤ F2-2

C	-0.360185	0.158190	-0.928148
N	-0.134485	1.377372	-0.996444
C	1.684824	2.698982	0.855488
C	2.049248	2.016683	-0.266716
H	-0.430610	1.930439	-1.803135
H	2.280627	2.594132	-1.164435
O	1.330242	3.261820	1.789632
O	-0.503381	-0.976708	-0.715020
H	2.437526	1.002866	-0.142182

➤ DF2-2

DF2-2a^{•+}:

C	1.672147	2.446125	0.258863
C	2.390214	1.846503	-0.754791
H	3.483512	1.803990	-0.669465
O	1.078766	2.941645	1.097089
H	1.844485	1.434962	-1.613819

DF2-2b:

C	-0.773659	0.563678	-0.697710
N	-0.463833	1.731621	-0.511439
H	-1.100259	2.440107	-0.160627
O	-0.915064	-0.586084	-0.924866

Points of figure 6 :

➤ TS3-0

C	-0.113379	0.579411	0.080093
N	-0.359584	1.458833	1.033919
C	2.316589	2.124289	-0.781690
C	2.901774	0.968312	-0.368844
C	2.266591	-0.165482	0.146758
N	0.976426	-0.365735	0.376576
H	-1.320301	1.828683	1.078726
H	3.990494	0.958486	-0.480855
H	2.917192	-1.006611	0.396326
O	1.895136	3.124324	-1.155253
O	-0.591833	0.604577	-1.058499
H	0.688367	-1.285112	0.717755

➤ I3-1

C	0.113557	0.758574	0.284259
N	-1.083649	0.552102	0.725190
C	1.944029	2.022824	-0.801759
C	2.793660	0.864947	-0.530758
C	2.295470	-0.261132	0.094854
N	1.004980	-0.293881	0.474429
H	-1.701555	1.361021	0.564605
H	3.835200	0.919604	-0.847290
H	2.898410	-1.145925	0.304917
O	2.235285	3.041390	-1.348712
O	0.560938	1.867237	-0.321874
H	0.599647	-1.113797	0.940749

➤ TS3-1

C	-0.278054	1.181764	0.122838
N	-1.117849	0.855095	0.906304
C	2.044289	2.054740	-0.783167
C	2.806915	0.862789	-0.563142
C	2.335631	-0.406706	-0.118695
N	1.083105	-0.578250	0.184084
H	-1.845126	1.366385	1.401766
H	3.875086	1.010247	-0.741958
H	3.085514	-1.205042	-0.031934
O	2.265567	3.173169	-1.052024
O	0.346536	1.754015	-0.783778
H	0.855146	-1.516239	0.543535

➤ F3-1

C	-0.625468	1.363817	-0.449659
N	-1.230732	0.643281	0.328985
C	2.781313	2.038093	-0.315317
C	2.804878	0.756693	-0.821049
C	2.240533	-0.302821	-0.043138
N	1.609681	0.015813	1.056161
H	-1.755344	0.957477	1.144416
H	3.281372	0.621169	-1.796532
H	2.374427	-1.322666	-0.430677
O	2.842016	3.104557	0.093366
O	0.014885	1.897277	-1.284517
H	1.197346	-0.811345	1.512050

➤ DF3-1

DF3-1a^{•+}

C	1.664772	2.295340	0.000000
C	2.740749	1.406218	0.000000
C	2.425126	0.018669	0.000000
N	1.143014	-0.264874	0.000000
H	3.749047	1.834817	0.000000
H	3.254195	-0.703585	0.000000
O	0.844319	3.087141	0.000000
H	0.960532	-1.281259	0.000000

DF3-1b :

C	-0.773659	0.563678	-0.697710
N	-0.463833	1.731621	-0.511439
H	-1.100259	2.440107	-0.160627
O	-0.915064	-0.586084	-0.924866

À partir d'ici, il faut ajouter DF3-1b :

➤ TS3-2

C	1.775710	2.630198	0.955705
C	2.888875	1.942879	0.746512
C	2.277934	-0.657633	-0.466550
N	1.192117	-0.957254	-0.686033
H	3.894834	2.290071	0.983226
H	3.332831	-0.480014	-0.304089
O	0.693981	3.070412	1.058939
H	0.206456	-1.152910	-0.852691

➤ F3-2

C	2.430091	2.985032	-0.472123
C	3.049076	1.786085	-0.277060
C	1.533906	-0.719761	0.229732
N	0.999888	-1.736568	0.417882
H	4.142429	1.738070	-0.313055
H	2.404774	0.835027	-0.077117
O	1.841760	3.958349	-0.623904
H	0.536016	-2.621574	0.582541

➤ DF3-2

DF3-2a^{•+}:

C	1.672147	2.446125	0.258863
C	2.390214	1.846503	-0.754791
H	3.483512	1.803990	-0.669465
O	1.078766	2.941645	1.097089
H	1.844485	1.434962	-1.613819

DF3-1b:

C	1.579283	-0.727918	0.279637
N	0.996986	-1.742252	0.415093
H	0.493541	-2.607734	0.535425