

Supporting Information

Peptide Bond Formation Mechanism Catalyzed by Ribosome

Katarzyna Świderek,^{1,2} Sergio Marti,¹ Iñaki Tuñón,³ Vicent Moliner,¹ Juan Bertrán⁴

1. Departament de Química Física i Analítica; Universitat Jaume I, 12071 Castellón (Spain)

2. Institute of Applied Radiation Chemistry, Lodz University of Technology, 90-924 Lodz, (Poland)

3. Departament de Química Física, Universitat de València, 46100 Burjasot, (Spain)

4. Departament de Química; Universitat Autònoma de Barcelona, 08193 Bellaterra, (Spain)

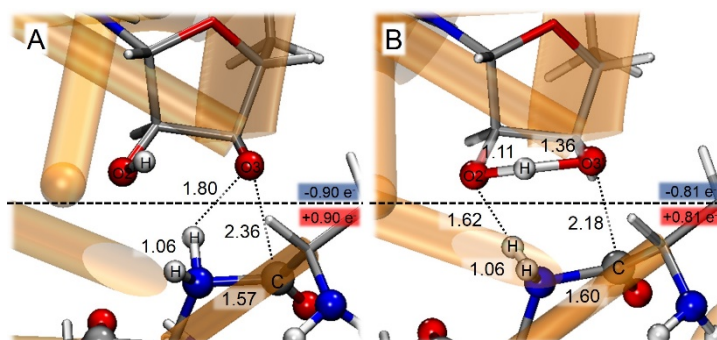


Figure S1. Geometries of the four-(A) and six- (B) membered ring TSs obtained for the peptide bond formation catalysed by ribosome, computed at M06-2X/MM level. Distances are reported in Å and charges of the two fragments in a.u.

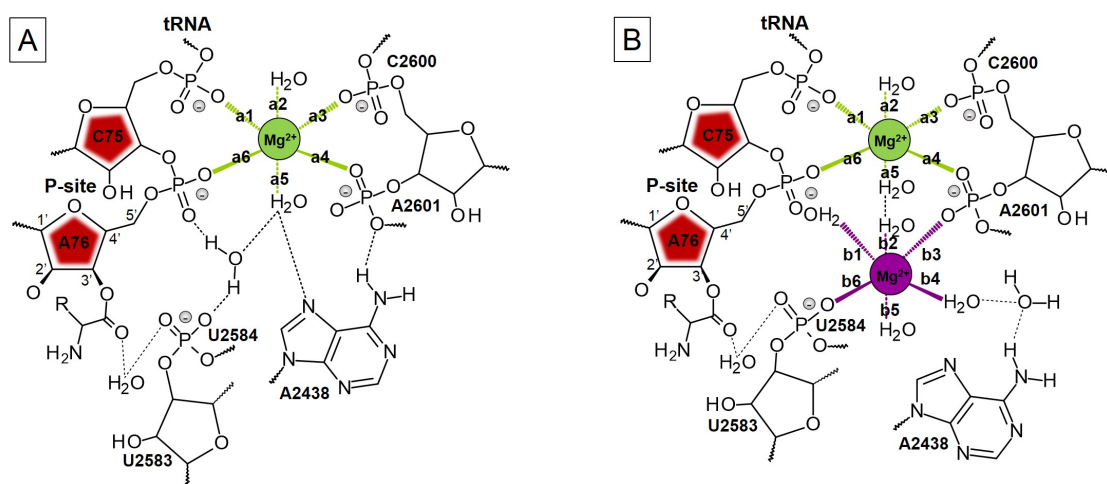


Figure S2. Schematic representation of the PTC without (A) and with an additional Mg²⁺ (B).

Table S1. Interatomic distances (in Å) defining the coordination sphere of Mg²⁺ ions in MC and TS. Models A and B as shown in Figure S2.

	a1	a2	a3	a4	a5	a6
MC^A	1.89 ± 0.04	2.08 ± 0.08	1.93 ± 0.05	1.89 ± 0.04	2.07 ± 0.07	1.94 ± 0.05
TS^A	1.89 ± 0.04	2.07 ± 0.09	1.92 ± 0.05	1.90 ± 0.05	2.08 ± 0.08	1.91 ± 0.05
MC^B	1.87 ± 0.04	2.01 ± 0.05	1.92 ± 0.05	1.90 ± 0.04	2.29 ± 0.20	1.91 ± 0.04
TS^B	1.86 ± 0.04	2.01 ± 0.06	1.91 ± 0.05	1.90 ± 0.04	2.27 ± 0.15	1.91 ± 0.05
	b1	b2	b3	b4	b5	b6
MC^B	1.97 ± 0.06	2.00 ± 0.06	1.88 ± 0.04	1.98 ± 0.05	2.51 ± 0.74	1.88 ± 0.04
TS^B	1.94 ± 0.04	1.97 ± 0.05	1.87 ± 0.04	1.97 ± 0.05	5.23 ± 0.64	1.86 ± 0.04

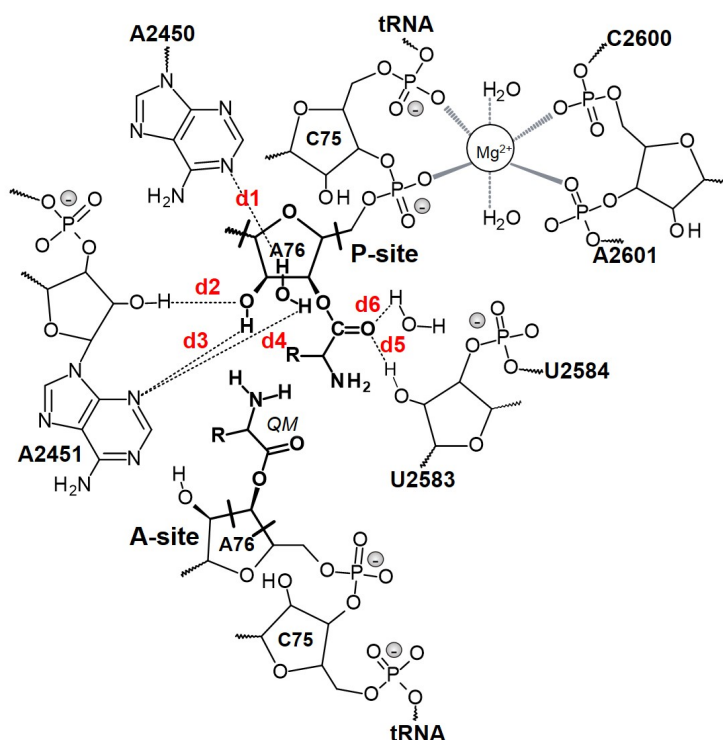


Figure S3. Schematic representation of the active site with labels for key intermolecular interactions.

Table S2. Average key interatomic distances in RC, ZW and TS-8, as depicted in Figure S3.

	Ribosome			Ribosome +Mg ²⁺		
	RC	ZW	TS	RC	ZW	TS
d1	1.91±0.15	2.01±0.15	2.04±0.11	3.33±1.04	2.02±0.13	2.03±0.12
d2	4.19±0.28	3.68±0.99	2.98±0.20	3.15±0.10	3.97±0.71	1.88±0.24
d3	3.25±0.12	3.39±0.13	3.38±0.11	3.72±0.11	3.30±0.12	3.34±0.11
d4	3.97±0.15	3.79±0.12	3.89±0.10	1.97±0.13	3.66±0.11	3.82±0.10
d5	2.64±0.17	2.46±0.15	2.49±0.19	2.33±0.19	2.03±0.24	2.43±0.19
d6	2.06±0.29	1.86±0.19	1.88±0.16	-	-	-

Figure S4. Representation of the dipole moments of the QM subsystem in RC and TS-8.

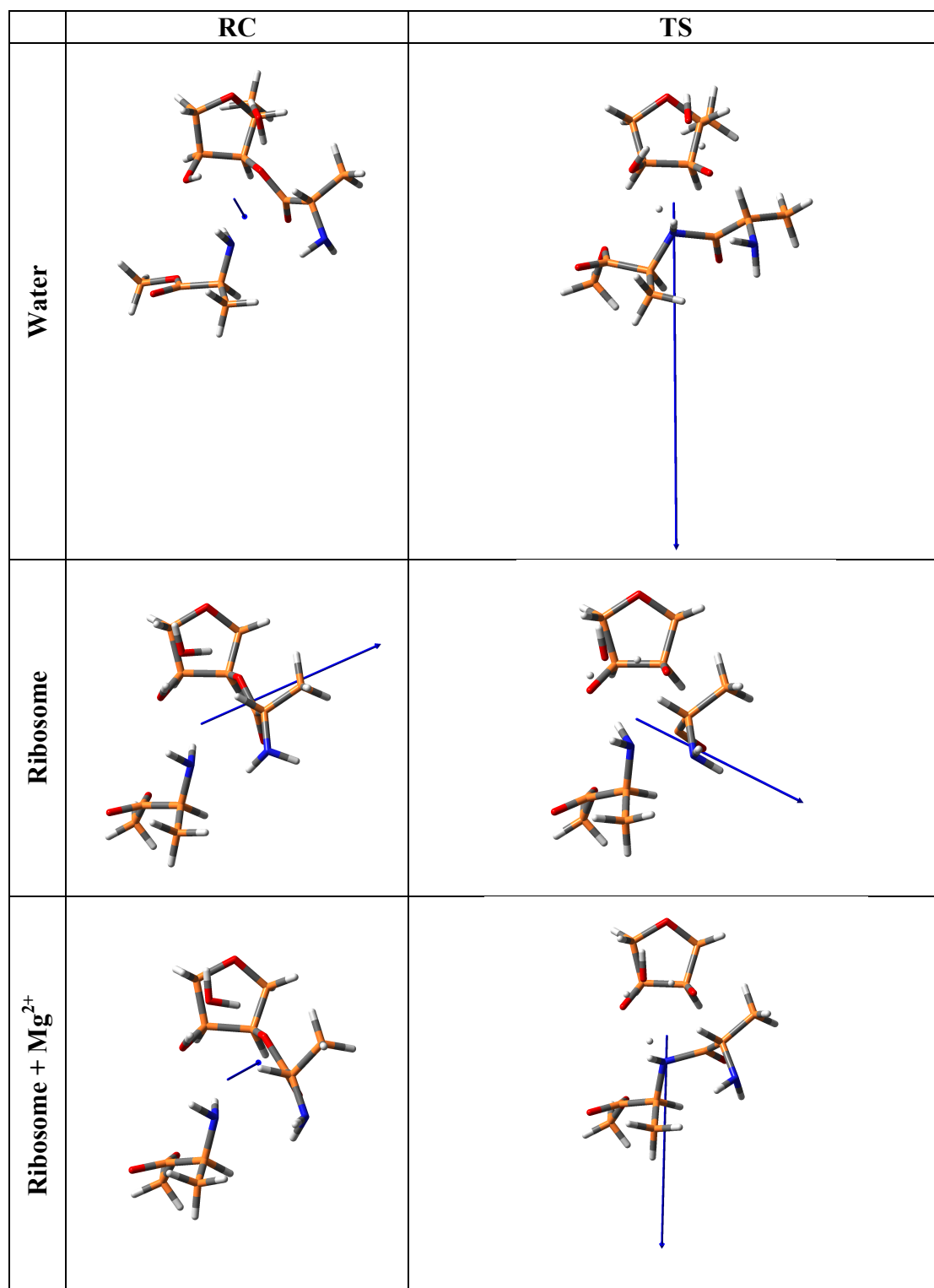


Table S3. Cartesian coordinates of QM sub-set of atoms for the TS-4, TS-6 and TS-8 obtained in the ribosome without (A) and with an additional Mg²⁺ (B).

TS-4

C	-15.92657000	-2.62748000	11.26598000
H	-16.61958000	-2.65204000	10.42602000
O	-16.22568000	-3.77638000	12.10356000
C	-16.05260000	-3.45699000	13.45830000
H	-16.96861000	-3.71985000	14.00388000
C	-16.23632000	-1.40649000	12.15795000
H	-15.61488000	-0.54983000	11.84990000
C	-15.82201000	-1.93932000	13.57266000
H	-14.80686000	-1.65767000	13.86062000
O	-16.68241000	-1.39920000	14.58254000
H	-17.57334000	-1.68209000	14.27278000
O	-17.57428000	-1.06750000	12.23463000
N	-20.99582000	1.32861000	11.85111000
H	-21.24147000	1.74073000	12.74569000
H	-20.85623000	2.07546000	11.17928000
C	-19.87824000	0.38294000	11.85973000
H	-20.13102000	-0.44890000	12.52268000
C	-19.64530000	-0.13205000	10.44191000
H	-19.07551000	0.60263000	9.86708000
H	-20.61448000	-0.30360000	9.96955000
H	-19.04791000	-1.04036000	10.47719000
C	-18.60031000	1.05403000	12.35769000
O	-17.96029000	1.87165000	11.78728000
C	-14.48847000	2.47772000	16.07291000
H	-13.57106000	1.94998000	15.80134000
O	-15.50885000	1.69375000	15.44639000
N	-18.20422000	0.81471000	13.85793000
H	-17.49214000	0.06233000	13.63333000
H	-18.93908000	0.32127000	14.38987000
C	-17.73053000	2.02757000	14.58045000
H	-17.13287000	2.57403000	13.84804000
C	-18.91901000	2.85261000	15.06095000
H	-19.43415000	2.34276000	15.87919000
H	-19.61331000	3.04560000	14.23871000
H	-18.57040000	3.81784000	15.43262000
C	-16.80363000	1.77990000	15.79729000
O	-17.18799000	1.80430000	16.93685000
H	-14.53695000	3.40456000	15.70061000
H	-14.43625000	2.68330000	17.05016000
H	-15.31670000	-3.98242000	13.88534000
H	-14.98890000	-2.69466000	10.92503000

TS-6

C	-15.98752000	-2.72662000	11.21383000
H	-16.66559000	-2.80759000	10.36580000
O	-16.25294000	-3.84505000	12.08603000
C	-16.03571000	-3.47015000	13.42399000
H	-16.94392000	-3.68227000	14.00175000
C	-16.30443000	-1.49947000	12.07059000
H	-15.82298000	-0.59442000	11.67617000
C	-15.78520000	-1.94849000	13.48136000
H	-14.75898000	-1.64761000	13.69893000
O	-16.68250000	-1.37198000	14.41662000
H	-17.48663000	-1.41805000	13.65118000
O	-17.66959000	-1.27907000	12.31152000
N	-20.72104000	1.40407000	11.88732000
H	-21.03920000	1.73907000	12.78929000
H	-20.34517000	2.18985000	11.36747000
C	-19.77100000	0.28983000	11.91802000
H	-20.15764000	-0.48061000	12.58986000
C	-19.64428000	-0.27322000	10.50381000
H	-19.01646000	0.38154000	9.89264000
H	-20.64472000	-0.32782000	10.06957000
H	-19.18104000	-1.25674000	10.52492000
C	-18.40292000	0.77323000	12.41564000
O	-17.67652000	1.51896000	11.84027000
C	-14.57524000	2.49277000	16.06370000
H	-13.67556000	1.94750000	15.76935000
O	-15.62802000	1.72300000	15.47575000
N	-18.15784000	0.73371000	13.99329000
H	-17.32603000	0.08765000	14.12304000
H	-18.92889000	0.26361000	14.49794000
C	-17.82574000	2.05220000	14.59592000
H	-17.22686000	2.55583000	13.83319000
C	-19.05648000	2.85772000	14.97083000
H	-19.59058000	2.39185000	15.80266000
H	-19.71651000	2.96935000	14.10767000
H	-18.75094000	3.85809000	15.28227000
C	-16.91469000	1.90192000	15.82743000
O	-17.29880000	2.02380000	16.96005000
H	-14.61687000	3.42393000	15.70147000
H	-14.51646000	2.68842000	17.04261000
H	-15.29737000	-4.00194000	13.83879000
H	-15.03984000	-2.74840000	10.89536000

(A) TS-8

C	-15.95036000	-2.67049000	11.07572000
H	-16.56935000	-2.73628000	10.18201000
O	-16.25514000	-3.82376000	11.90230000
C	-16.12410000	-3.49843000	13.26250000
H	-17.04382000	-3.79765000	13.77288000
C	-16.38034000	-1.47088000	11.93999000
H	-15.86297000	-0.55551000	11.62550000
C	-15.96270000	-1.96848000	13.35921000
H	-14.94197000	-1.65034000	13.59114000
O	-16.80241000	-1.48740000	14.40685000
H	-17.70732000	-1.96921000	14.23697000
O	-17.76700000	-1.24144000	11.90687000
N	-20.64005000	1.42946000	11.98360000
H	-20.32132000	2.17601000	11.37169000
H	-21.61751000	1.25976000	11.76394000
C	-19.82779000	0.22813000	11.73864000
H	-20.20068000	-0.57759000	12.38025000
C	-19.80487000	-0.22920000	10.28006000
H	-19.12531000	0.40229000	9.70032000
H	-20.81252000	-0.15269000	9.86059000
H	-19.44871000	-1.25547000	10.19845000
C	-18.42924000	0.63205000	12.20558000
O	-17.74545000	1.44355000	11.65132000
C	-14.58852000	2.40867000	16.02709000
H	-13.66581000	1.88434000	15.76828000
O	-15.59590000	1.62146000	15.37567000
N	-18.21977000	0.57861000	13.78432000
H	-17.47646000	-0.15888000	13.94621000
H	-19.04989000	0.19120000	14.26180000
C	-17.79463000	1.87029000	14.39979000
H	-17.17288000	2.34380000	13.63677000
C	-18.99839000	2.72842000	14.76131000
H	-19.52263000	2.29791000	15.61829000
H	-19.67491000	2.79369000	13.90626000
H	-18.66994000	3.73165000	15.03803000
C	-16.91128000	1.70763000	15.66631000
O	-17.33884000	1.75732000	16.78986000
O	-18.97152000	-2.41238000	13.59456000
H	-19.20891000	-3.34376000	13.45817000
H	-18.43825000	-1.95850000	12.64843000
H	-14.63215000	3.33473000	15.65222000
H	-14.55577000	2.62106000	17.00372000
H	-15.38555000	-3.97794000	13.73642000
H	-14.98706000	-2.69250000	10.80820000

(B) TS-8-Mg

C	-15.74648000	-2.77968000	10.75632000
H	-16.40836000	-2.87273000	9.89235000
O	-15.94190000	-3.94623000	11.56926000
C	-15.83524000	-3.63746000	12.94361000
H	-16.76074000	-3.95015000	13.43854000
C	-16.17324000	-1.60441000	11.64437000
H	-15.65789000	-0.67716000	11.36210000
C	-15.71286000	-2.10201000	13.04867000
H	-14.69956000	-1.75892000	13.27024000
O	-16.55850000	-1.59237000	14.07055000
H	-17.47220000	-2.05614000	13.90985000
O	-17.55227000	-1.35233000	11.62080000
N	-20.16733000	1.76168000	11.42206000
H	-20.72319000	1.91808000	12.25600000
H	-19.49528000	2.52353000	11.35332000
C	-19.45774000	0.46001000	11.41626000
H	-19.95544000	-0.24353000	12.09211000
C	-19.49474000	-0.11966000	10.00448000
H	-18.87596000	0.48902000	9.33808000
H	-20.53189000	-0.09396000	9.65806000
H	-19.11602000	-1.14030000	9.99081000
C	-18.01528000	0.69391000	11.89199000
O	-17.20996000	1.32198000	11.26334000
C	-13.93151000	2.43708000	15.47505000
H	-13.03871000	1.91707000	15.13620000
O	-15.01754000	1.72939000	14.81350000
N	-17.76230000	0.62599000	13.42485000
H	-17.07110000	-0.17014000	13.58994000
H	-18.59043000	0.27760000	13.93528000
C	-17.27146000	1.91247000	14.04577000
H	-16.73884000	2.43082000	13.24848000
C	-18.44897000	2.72529000	14.55886000
H	-18.90957000	2.22914000	15.41625000
H	-19.17908000	2.89029000	13.76202000
H	-18.09611000	3.70248000	14.88746000
C	-16.27810000	1.70030000	15.22801000
O	-16.65274000	1.60920000	16.37013000
O	-18.77156000	-2.52134000	13.31076000
H	-18.92766000	-3.45120000	13.08495000
H	-18.19892000	-2.00386000	12.34193000
H	-13.99724000	3.38063000	15.15042000
H	-13.84819000	2.59566000	16.45887000
H	-15.09667000	-4.14791000	13.38402000
H	-14.79460000	-2.71633000	10.45647000