

Supporting Information

Computational Investigation of the Control of Thermodynamics and Microkinetics of the Reductive Amination Reaction by Solvent Coordination and a Co-Catalyst

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Selected Bond Lengths and NBO Charges for the Compounds

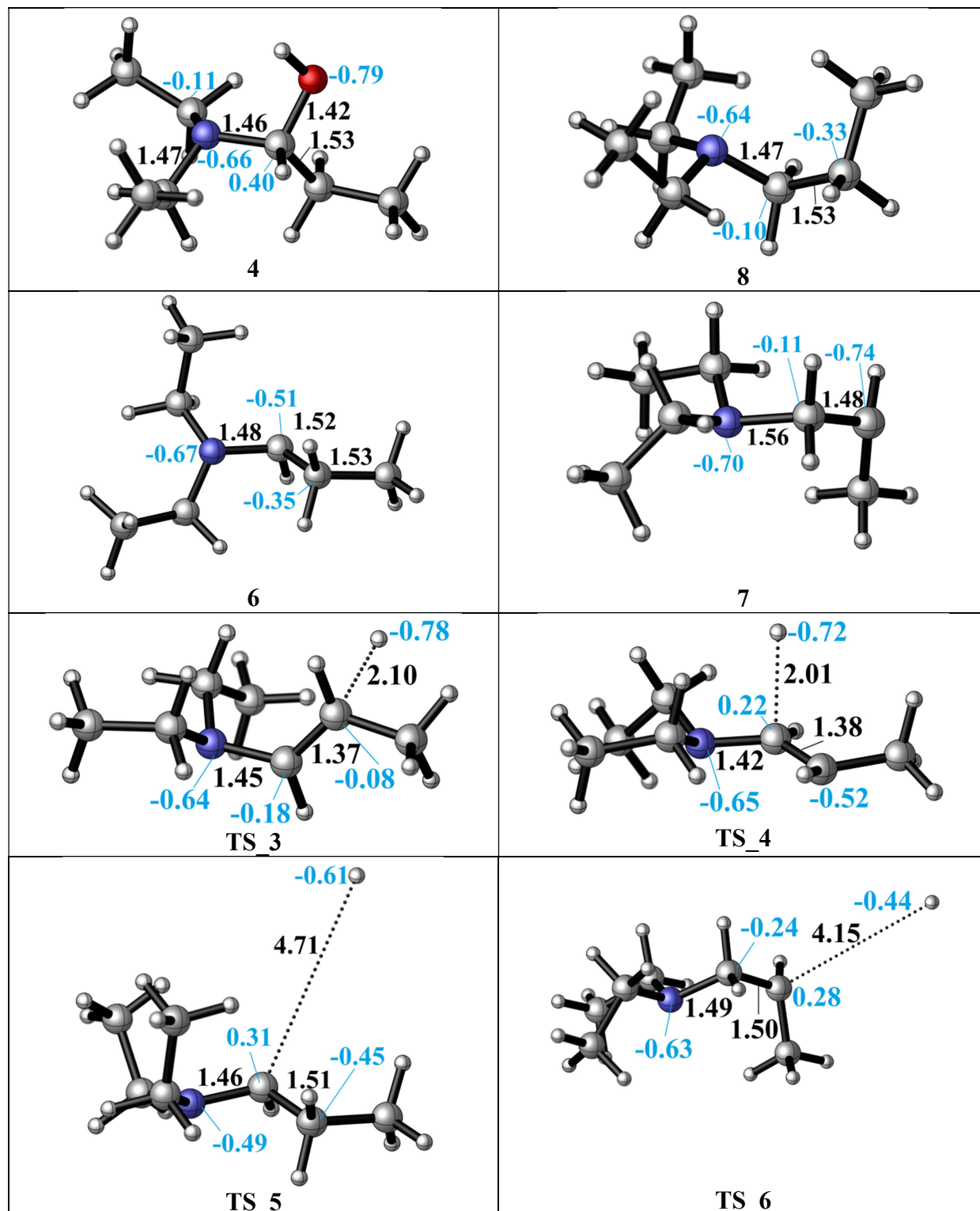


Figure S1. The selected bond lengths (in Å, black) and NBO charges (blue) of the transition state and intermediate structures for reductive amination reaction in neutral media.

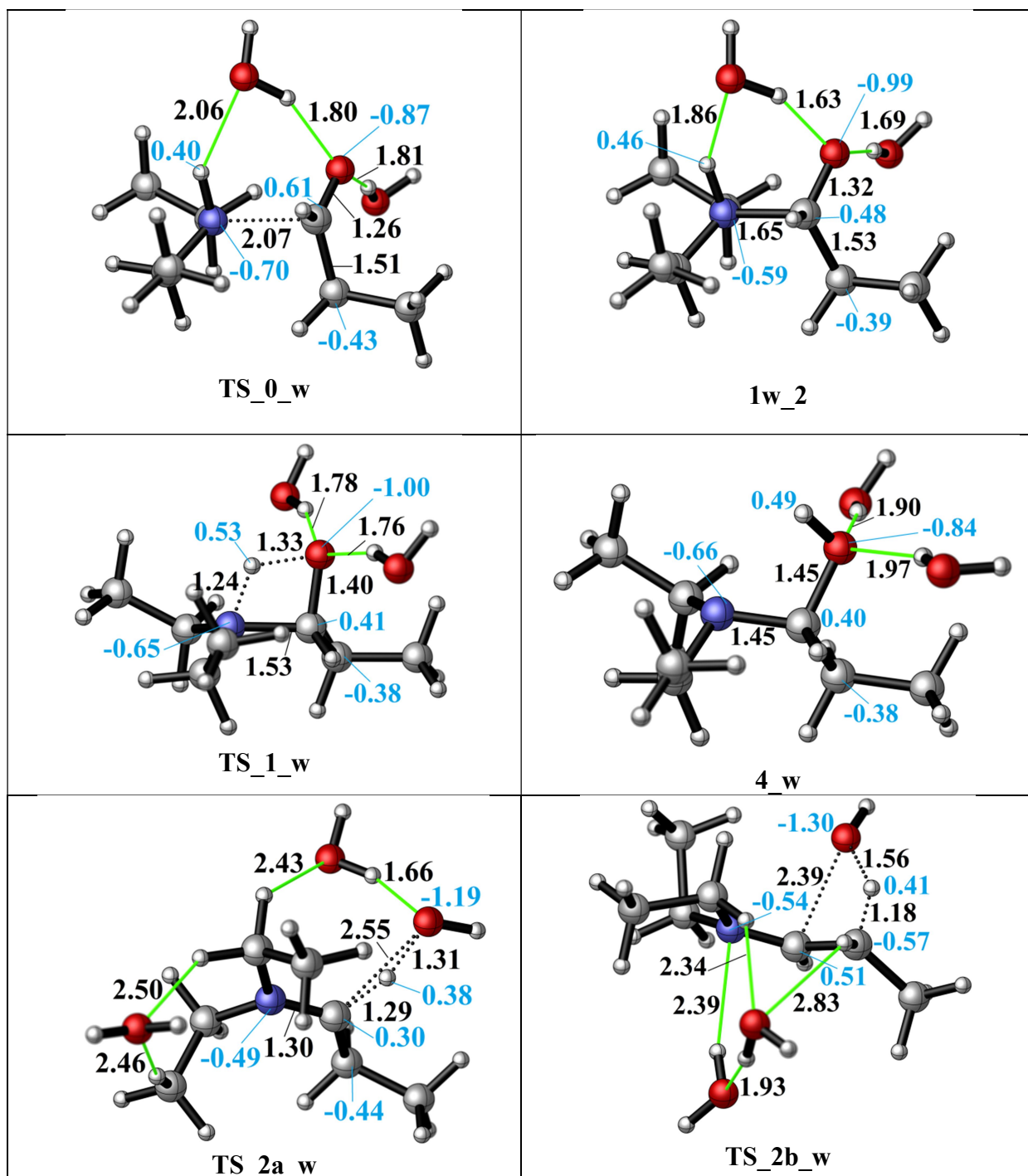


Figure S2. The selected bond lengths (in Å, black) and NBO charges (blue) of the transition state and intermediate structures for reductive amination reaction in neutral media with explicit water assistance.

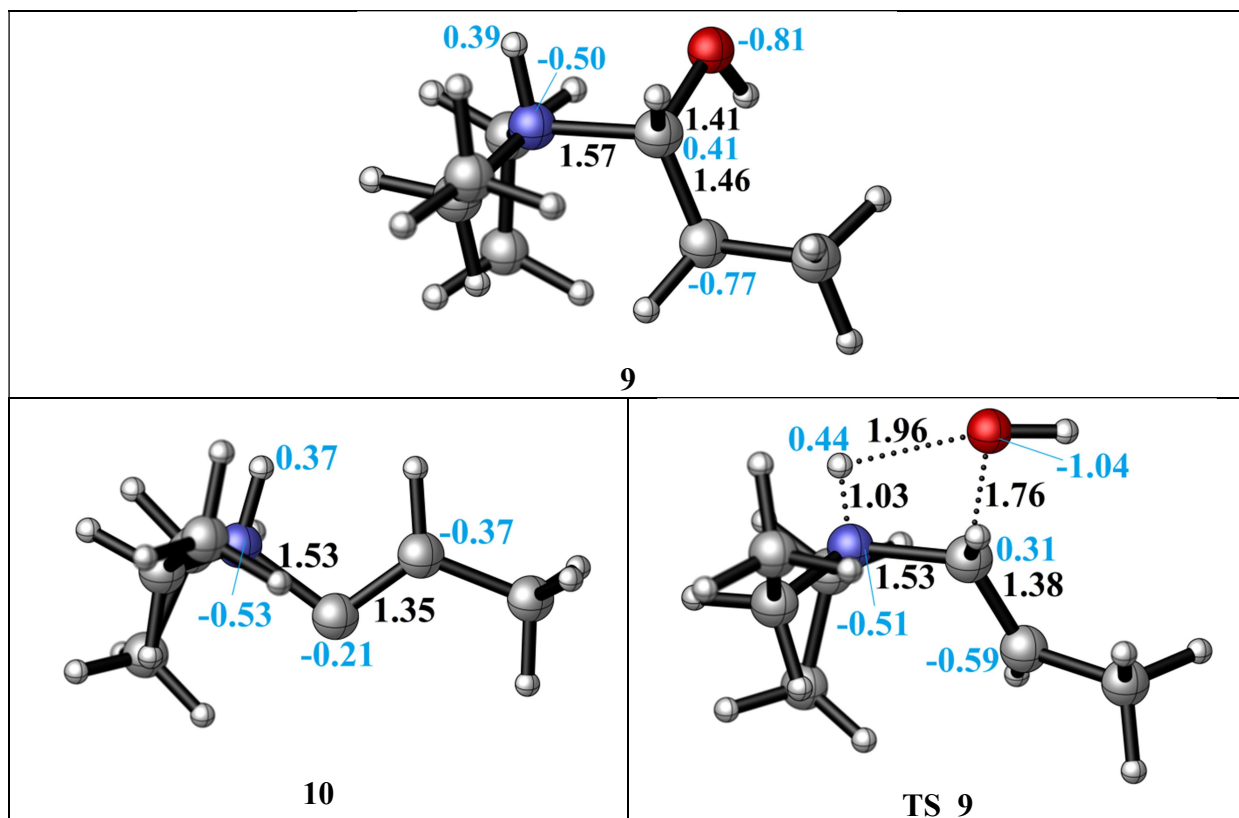


Figure S3. The selected bond lengths (in Å, black) and NBO charges (blue) of the transition state and intermediate structures for reductive amination reaction in low pH.

	1..2	TS_1	4	TS_2a	TS_2b	5a	5b	5c	TS_3	TS_4	6	7	TS_5	TS_6	TS_7	8
Gas phase	4.2	33.3	2.1	48.9	48.9	33.4	2.1	-71.3	0.2	-1.2	-28.1	-25.9	-134.9	-125.2	-46.9	-14.7
DMF	9.1	32.4	5.6	41.1	45.1	26.8	1.3	-53.6	29.4	28.2	11.4	12.1	-6.7	38.0	-150	-15.1
Decane	7.6	34.1	3.7	45.7	47.4	30.7	1.7	-62.2	19.2	17.8	-5.8	-4.7	-45.7	-11.5	-74.9	-15.3

Table S1. Relative Gibbs free energies of the transition states and intermediate structures for reductive amination reaction in neutral media calculated in the gas phase and implicit solvent (in DMF and decane).

	1_w..2	TS_0_w	1w_2	TS_1_w	4_w	TS_2a_w	TS_2b_w	TS_2c_w	5a_w	5b_w	5c_w	8
Gas phase	2.5	7.3	8.6	24.3	0.9	34.0	49.6	28.1	30.4	-2.1	-81.8	-21.5
DMF	7.5	10.6	8.4	26.2	4.2	33.1	45.2	25.8	27.2	-3.1	-53.6	-27.3
Decane	9.6	13.7	13.6	30.2	7.4	38.6	53.2	32.1	34.1	2.5	-62.6	-19.3

Table S2. Relative Gibbs free energies of the transition states and intermediate structures for reductive amination reaction in neutral media with explicit water assistance calculated in the gas phase and implicit solvent (in DMF and decane).

	1_H⁺ .. 2	3+2	3 .. 2	TS_10	9	TS_11	10	TS_9	5b
Gas phase	-19.0	11.1	15.5	72.5	71.4	58.0	54.0	68.5	2.2
DMF	-10	11.6	18.1	66.8	61.6	48.7	41.1	64.0	1.7
Decane	-14	11.5	16.6	71.0	68.4	54.7	49.5	66.9	1.3

Table S3. Relative Gibbs free energies of the transition states and intermediate structures for reductive amination reaction following the keto-enol tautomerization in the presence of an acid calculated in the gas phase and implicit solvent (in DMF and decane).

	1 + 2_H⁺	1 .. 2_H⁺	TS_12	11	TS_13	TS_14	5c
Gas phase	-61.6	-69.2	-24.0	-62.9	-27.1	-51.9	-71.3
DMF	-52.8	-44.5	-1.7	-42.1	-4.1	-33.2	-53.6
Decane	-56.7	-56.6	-12.2	-51.8	-15.2	-41.5	-62.2

Table S4. Relative Gibbs free energies of the transition states and intermediate structures for reductive amination reaction in the presence of an acid as a co-catalyst for Case A and Case B calculated in the gas phase and implicit solvent (in DMF and decane).

Free energies and thermal corrections of the transition states and intermediate structures for reductive amination reaction

1

Zero-point correction= (Hartree/Particle)	0.085349
Thermal correction to Energy=	0.090302
Thermal correction to Enthalpy=	0.091247
Thermal correction to Gibbs Free Energy=	0.058093
Sum of electronic and zero-point Energies=	-192.560172
Sum of electronic and thermal Energies=	-192.555218
Sum of electronic and thermal Enthalpies=	-192.554274
Sum of electronic and thermal Free Energies=	-192.587428

2

Zero-point correction= (Hartree/Particle)	0.151522
Thermal correction to Energy=	0.158312
Thermal correction to Enthalpy=	0.159257
Thermal correction to Gibbs Free Energy=	0.121372
Sum of electronic and zero-point Energies=	-213.022772
Sum of electronic and thermal Energies=	-213.015982
Sum of electronic and thermal Enthalpies=	-213.015038
Sum of electronic and thermal Free Energies=	-213.052922

1..2

Zero-point correction= (Hartree/Particle)	0.237742
Thermal correction to Energy=	0.251508
Thermal correction to Enthalpy=	0.252452
Thermal correction to Gibbs Free Energy=	0.192565
Sum of electronic and zero-point Energies=	-405.588531
Sum of electronic and thermal Energies=	-405.574764
Sum of electronic and thermal Enthalpies=	-405.573820
Sum of electronic and thermal Free Energies=	-405.633707

4

Zero-point correction= (Hartree/Particle)	0.241899
Thermal correction to Energy=	0.253594
Thermal correction to Enthalpy=	0.254538
Thermal correction to Gibbs Free Energy=	0.204816
Sum of electronic and zero-point Energies=	-405.599881
Sum of electronic and thermal Energies=	-405.588187
Sum of electronic and thermal Enthalpies=	-405.587242

Sum of electronic and thermal Free Energies= -405.636965

5a

Zero-point correction= 0.212529
(Hartree/Particle)
Thermal correction to Energy= 0.222896
Thermal correction to Enthalpy= 0.223840
Thermal correction to Gibbs Free Energy= 0.176943
Sum of electronic and zero-point Energies= -329.280828
Sum of electronic and thermal Energies= -329.270461
Sum of electronic and thermal Enthalpies= -329.269517
Sum of electronic and thermal Free Energies= -329.316414

5b

Zero-point correction= 0.212816
(Hartree/Particle)
Thermal correction to Energy= 0.223103
Thermal correction to Enthalpy= 0.224047
Thermal correction to Gibbs Free Energy= 0.177874
Sum of electronic and zero-point Energies= -329.331386
Sum of electronic and thermal Energies= -329.321099
Sum of electronic and thermal Enthalpies= -329.320155
Sum of electronic and thermal Free Energies= -329.366328

5c

Zero-point correction= 0.227197
(Hartree/Particle)
Thermal correction to Energy= 0.237652
Thermal correction to Enthalpy= 0.238597
Thermal correction to Gibbs Free Energy= 0.191530
Sum of electronic and zero-point Energies= -329.709831
Sum of electronic and thermal Energies= -329.699375
Sum of electronic and thermal Enthalpies= -329.698431
Sum of electronic and thermal Free Energies= -329.745497

6

Zero-point correction= 0.218929
(Hartree/Particle)
Thermal correction to Energy= 0.229676
Thermal correction to Enthalpy= 0.230620
Thermal correction to Gibbs Free Energy= 0.182968
Sum of electronic and zero-point Energies= -329.871368
Sum of electronic and thermal Energies= -329.860621
Sum of electronic and thermal Enthalpies= -329.859677
Sum of electronic and thermal Free Energies= -329.907330

7

Zero-point correction=	0.218630
(Hartree/Particle)	
Thermal correction to Energy=	0.229321
Thermal correction to Enthalpy=	0.230265
Thermal correction to Gibbs Free Energy=	0.182886
Sum of electronic and zero-point Energies=	-329.868127
Sum of electronic and thermal Energies=	-329.857436
Sum of electronic and thermal Enthalpies=	-329.856492
Sum of electronic and thermal Free Energies=	-329.903871

8

Zero-point correction=	0.236890
(Hartree/Particle)	
Thermal correction to Energy=	0.247539
Thermal correction to Enthalpy=	0.248484
Thermal correction to Gibbs Free Energy=	0.200831
Sum of electronic and zero-point Energies=	-330.518445
Sum of electronic and thermal Energies=	-330.507795
Sum of electronic and thermal Enthalpies=	-330.506850
Sum of electronic and thermal Free Energies=	-330.554504

TS_1

Zero-point correction=	0.237190
(Hartree/Particle)	
Thermal correction to Energy=	0.248659
Thermal correction to Enthalpy=	0.249603
Thermal correction to Gibbs Free Energy=	0.199818
Sum of electronic and zero-point Energies=	-405.546564
Sum of electronic and thermal Energies=	-405.535095
Sum of electronic and thermal Enthalpies=	-405.534151
Sum of electronic and thermal Free Energies=	-405.583936

TS_2a

Zero-point correction=	0.235933
(Hartree/Particle)	
Thermal correction to Energy=	0.248488
Thermal correction to Enthalpy=	0.249432
Thermal correction to Gibbs Free Energy=	0.197913
Sum of electronic and zero-point Energies=	-405.524475
Sum of electronic and thermal Energies=	-405.511921
Sum of electronic and thermal Enthalpies=	-405.510976
Sum of electronic and thermal Free Energies=	-405.562496

TS_2b

Zero-point correction=	0.235547
(Hartree/Particle)	
Thermal correction to Energy=	0.247675
Thermal correction to Enthalpy=	0.248620
Thermal correction to Gibbs Free Energy=	0.198201
Sum of electronic and zero-point Energies=	-405.525038
Sum of electronic and thermal Energies=	-405.512910
Sum of electronic and thermal Enthalpies=	-405.511965
Sum of electronic and thermal Free Energies=	-405.562384

TS_3

Zero-point correction=	0.212840
(Hartree/Particle)	
Thermal correction to Energy=	0.223670
Thermal correction to Enthalpy=	0.224615
Thermal correction to Gibbs Free Energy=	0.177393
Sum of electronic and zero-point Energies=	-329.826768
Sum of electronic and thermal Energies=	-329.815938
Sum of electronic and thermal Enthalpies=	-329.814994
Sum of electronic and thermal Free Energies=	-329.862215

TS_4

Zero-point correction=	0.213594
(Hartree/Particle)	
Thermal correction to Energy=	0.224274
Thermal correction to Enthalpy=	0.225218
Thermal correction to Gibbs Free Energy=	0.178328
Sum of electronic and zero-point Energies=	-329.829301
Sum of electronic and thermal Energies=	-329.818620
Sum of electronic and thermal Enthalpies=	-329.817676
Sum of electronic and thermal Free Energies=	-329.864567

TS_5

Zero-point correction=	0.222958
(Hartree/Particle)	
Thermal correction to Energy=	0.235123
Thermal correction to Enthalpy=	0.236067
Thermal correction to Gibbs Free Energy=	0.185221
Sum of electronic and zero-point Energies=	-330.302066
Sum of electronic and thermal Energies=	-330.289901
Sum of electronic and thermal Enthalpies=	-330.288957
Sum of electronic and thermal Free Energies=	-330.339803

TS_6

Zero-point correction=	0.222299
(Hartree/Particle)	
Thermal correction to Energy=	0.234377
Thermal correction to Enthalpy=	0.235322
Thermal correction to Gibbs Free Energy=	0.184221
Sum of electronic and zero-point Energies=	-330.286258
Sum of electronic and thermal Energies=	-330.274179
Sum of electronic and thermal Enthalpies=	-330.273235
Sum of electronic and thermal Free Energies=	-330.324335

TS_7

Zero-point correction=	0.222964
(Hartree/Particle)	
Thermal correction to Energy=	0.235039
Thermal correction to Enthalpy=	0.235984
Thermal correction to Gibbs Free Energy=	0.184901
Sum of electronic and zero-point Energies=	-330.305654
Sum of electronic and thermal Energies=	-330.293578
Sum of electronic and thermal Enthalpies=	-330.292634
Sum of electronic and thermal Free Energies=	-330.343717

1_w

Zero-point correction=	0.134452
(Hartree/Particle)	
Thermal correction to Energy=	0.146576
Thermal correction to Enthalpy=	0.147520
Thermal correction to Gibbs Free Energy=	0.094394
Sum of electronic and zero-point Energies=	-345.077930
Sum of electronic and thermal Energies=	-345.065807
Sum of electronic and thermal Enthalpies=	-345.064863
Sum of electronic and thermal Free Energies=	-345.117989

1w..2

Zero-point correction=	0.288043
(Hartree/Particle)	
Thermal correction to Energy=	0.308158
Thermal correction to Enthalpy=	0.309103
Thermal correction to Gibbs Free Energy=	0.236771
Sum of electronic and zero-point Energies=	-558.115591
Sum of electronic and thermal Energies=	-558.095475
Sum of electronic and thermal Enthalpies=	-558.094531
Sum of electronic and thermal Free Energies=	-558.166862

1w_2

Zero-point correction=	0.292837
(Hartree/Particle)	
Thermal correction to Energy=	0.310149
Thermal correction to Enthalpy=	0.311093
Thermal correction to Gibbs Free Energy=	0.247712
Sum of electronic and zero-point Energies=	-558.112066
Sum of electronic and thermal Energies=	-558.094755
Sum of electronic and thermal Enthalpies=	-558.093811
Sum of electronic and thermal Free Energies=	-558.157192

4_w

Zero-point correction=	0.291361
(Hartree/Particle)	
Thermal correction to Energy=	0.309871
Thermal correction to Enthalpy=	0.310815
Thermal correction to Gibbs Free Energy=	0.244154
Sum of electronic and zero-point Energies=	-558.122304
Sum of electronic and thermal Energies=	-558.103795
Sum of electronic and thermal Enthalpies=	-558.102850
Sum of electronic and thermal Free Energies=	-558.169512

5a_w

Zero-point correction=	0.260838
(Hartree/Particle)	
Thermal correction to Energy=	0.278627
Thermal correction to Enthalpy=	0.279571
Thermal correction to Gibbs Free Energy=	0.213730
Sum of electronic and zero-point Energies=	-481.804653
Sum of electronic and thermal Energies=	-481.786863
Sum of electronic and thermal Enthalpies=	-481.785919
Sum of electronic and thermal Free Energies=	-481.851760

5b_w

Zero-point correction=	0.263056
(Hartree/Particle)	
Thermal correction to Energy=	0.279499
Thermal correction to Enthalpy=	0.280444
Thermal correction to Gibbs Free Energy=	0.218939
Sum of electronic and zero-point Energies=	-481.859412
Sum of electronic and thermal Energies=	-481.842968
Sum of electronic and thermal Enthalpies=	-481.842024
Sum of electronic and thermal Free Energies=	-481.903528

5c_w

Zero-point correction=	0.276565
(Hartree/Particle)	
Thermal correction to Energy=	0.293813
Thermal correction to Enthalpy=	0.294757
Thermal correction to Gibbs Free Energy=	0.229173
Sum of electronic and zero-point Energies=	-482.245461
Sum of electronic and thermal Energies=	-482.228214
Sum of electronic and thermal Enthalpies=	-482.227269
Sum of electronic and thermal Free Energies=	-482.292853

TS_0_w

Zero-point correction=	0.290158
(Hartree/Particle)	
Thermal correction to Energy=	0.308202
Thermal correction to Enthalpy=	0.309146
Thermal correction to Gibbs Free Energy=	0.243226
Sum of electronic and zero-point Energies=	-558.112346
Sum of electronic and thermal Energies=	-558.094302
Sum of electronic and thermal Enthalpies=	-558.093357
Sum of electronic and thermal Free Energies=	-558.159278

TS_1_w

Zero-point correction=	0.287629
(Hartree/Particle)	
Thermal correction to Energy=	0.305228
Thermal correction to Enthalpy=	0.306172
Thermal correction to Gibbs Free Energy=	0.241545
Sum of electronic and zero-point Energies=	-558.086110
Sum of electronic and thermal Energies=	-558.068511
Sum of electronic and thermal Enthalpies=	-558.067567
Sum of electronic and thermal Free Energies=	-558.132194

TS_2a_w

Zero-point correction=	0.282535
(Hartree/Particle)	
Thermal correction to Energy=	0.302110
Thermal correction to Enthalpy=	0.303054
Thermal correction to Gibbs Free Energy=	0.232475
Sum of electronic and zero-point Energies=	-558.066631
Sum of electronic and thermal Energies=	-558.047056
Sum of electronic and thermal Enthalpies=	-558.046112
Sum of electronic and thermal Free Energies=	-558.116691

TS_2b_w

Zero-point correction=	0.284207
(Hartree/Particle)	
Thermal correction to Energy=	0.303455
Thermal correction to Enthalpy=	0.304399
Thermal correction to Gibbs Free Energy=	0.236576
Sum of electronic and zero-point Energies=	-558.044193
Sum of electronic and thermal Energies=	-558.024945
Sum of electronic and thermal Enthalpies=	-558.024001
Sum of electronic and thermal Free Energies=	-558.091824

TS_2c_w

Zero-point correction=	0.289165
(Hartree/Particle)	
Thermal correction to Energy=	0.306285
Thermal correction to Enthalpy=	0.307229
Thermal correction to Gibbs Free Energy=	0.245228
Sum of electronic and zero-point Energies=	-558.082204
Sum of electronic and thermal Energies=	-558.065084
Sum of electronic and thermal Enthalpies=	-558.064140
Sum of electronic and thermal Free Energies=	-558.126141

1_H+

Zero-point correction=	0.098501
(Hartree/Particle)	
Thermal correction to Energy=	0.103597
Thermal correction to Enthalpy=	0.104541
Thermal correction to Gibbs Free Energy=	0.071127
Sum of electronic and zero-point Energies=	-192.852571
Sum of electronic and thermal Energies=	-192.847475
Sum of electronic and thermal Enthalpies=	-192.846530
Sum of electronic and thermal Free Energies=	-192.879945

3

Zero-point correction=	0.085485
(Hartree/Particle)	
Thermal correction to Energy=	0.090659
Thermal correction to Enthalpy=	0.091603
Thermal correction to Gibbs Free Energy=	0.057792
Sum of electronic and zero-point Energies=	-192.541993
Sum of electronic and thermal Energies=	-192.536819
Sum of electronic and thermal Enthalpies=	-192.535875
Sum of electronic and thermal Free Energies=	-192.569686

3..2

Zero-point correction=	0.238010
(Hartree/Particle)	
Thermal correction to Energy=	0.252007
Thermal correction to Enthalpy=	0.252951
Thermal correction to Gibbs Free Energy=	0.193581
Sum of electronic and zero-point Energies=	-405.571272
Sum of electronic and thermal Energies=	-405.557276
Sum of electronic and thermal Enthalpies=	-405.556332
Sum of electronic and thermal Free Energies=	-405.615701

9

Zero-point correction=	0.241288
(Hartree/Particle)	
Thermal correction to Energy=	0.252716
Thermal correction to Enthalpy=	0.253660
Thermal correction to Gibbs Free Energy=	0.204910
Sum of electronic and zero-point Energies=	-405.490156
Sum of electronic and thermal Energies=	-405.478729
Sum of electronic and thermal Enthalpies=	-405.477785
Sum of electronic and thermal Free Energies=	-405.526534

10

Zero-point correction=	0.212675
(Hartree/Particle)	
Thermal correction to Energy=	0.223006
Thermal correction to Enthalpy=	0.223950
Thermal correction to Gibbs Free Energy=	0.177513
Sum of electronic and zero-point Energies=	-329.248498
Sum of electronic and thermal Energies=	-329.238166
Sum of electronic and thermal Enthalpies=	-329.237222
Sum of electronic and thermal Free Energies=	-329.283659

TS_8

Zero-point correction=	0.250819
(Hartree/Particle)	
Thermal correction to Energy=	0.263702
Thermal correction to Enthalpy=	0.264646
Thermal correction to Gibbs Free Energy=	0.209943
Sum of electronic and zero-point Energies=	-405.897342
Sum of electronic and thermal Energies=	-405.884460
Sum of electronic and thermal Enthalpies=	-405.883516
Sum of electronic and thermal Free Energies=	-405.938219

TS_9

Zero-point correction=	0.239328
(Hartree/Particle)	
Thermal correction to Energy=	0.251114
Thermal correction to Enthalpy=	0.252058
Thermal correction to Gibbs Free Energy=	0.202321
Sum of electronic and zero-point Energies=	-405.494122
Sum of electronic and thermal Energies=	-405.482336
Sum of electronic and thermal Enthalpies=	-405.481392
Sum of electronic and thermal Free Energies=	-405.531128

TS_10

Zero-point correction=	0.239770
(Hartree/Particle)	
Thermal correction to Energy=	0.251137
Thermal correction to Enthalpy=	0.252081
Thermal correction to Gibbs Free Energy=	0.202996
Sum of electronic and zero-point Energies=	-405.488090
Sum of electronic and thermal Energies=	-405.476723
Sum of electronic and thermal Enthalpies=	-405.475779
Sum of electronic and thermal Free Energies=	-405.524863

TS_11

Zero-point correction=	0.234270
(Hartree/Particle)	
Thermal correction to Energy=	0.246693
Thermal correction to Enthalpy=	0.247637
Thermal correction to Gibbs Free Energy=	0.196589
Sum of electronic and zero-point Energies=	-405.510237
Sum of electronic and thermal Energies=	-405.497815
Sum of electronic and thermal Enthalpies=	-405.496871
Sum of electronic and thermal Free Energies=	-405.547918

2_H+

Zero-point correction=	0.166872
(Hartree/Particle)	
Thermal correction to Energy=	0.173773
Thermal correction to Enthalpy=	0.174717
Thermal correction to Gibbs Free Energy=	0.136558
Sum of electronic and zero-point Energies=	-213.383006
Sum of electronic and thermal Energies=	-213.376106
Sum of electronic and thermal Enthalpies=	-213.375161
Sum of electronic and thermal Free Energies=	-213.413320

1.. 2_H+

Zero-point correction=	0.253744
(Hartree/Particle)	
Thermal correction to Energy=	0.267427
Thermal correction to Enthalpy=	0.268372
Thermal correction to Gibbs Free Energy=	0.209590
Sum of electronic and zero-point Energies=	-405.968589
Sum of electronic and thermal Energies=	-405.954905
Sum of electronic and thermal Enthalpies=	-405.953961
Sum of electronic and thermal Free Energies=	-406.012743

1_H+..2

Zero-point correction=	0.257920
(Hartree/Particle)	
Thermal correction to Energy=	0.269274
Thermal correction to Enthalpy=	0.270219
Thermal correction to Gibbs Free Energy=	0.221868
Sum of electronic and zero-point Energies=	-405.953070
Sum of electronic and thermal Energies=	-405.941715
Sum of electronic and thermal Enthalpies=	-405.940771
Sum of electronic and thermal Free Energies=	-405.989122

11

Zero-point correction=	0.256815
(Hartree/Particle)	
Thermal correction to Energy=	0.268761
Thermal correction to Enthalpy=	0.269705
Thermal correction to Gibbs Free Energy=	0.219508
Sum of electronic and zero-point Energies=	-405.965383
Sum of electronic and thermal Energies=	-405.953438
Sum of electronic and thermal Enthalpies=	-405.952494
Sum of electronic and thermal Free Energies=	-406.002691

TS_12

Zero-point correction=	0.252168
(Hartree/Particle)	
Thermal correction to Energy=	0.264896
Thermal correction to Enthalpy=	0.265841
Thermal correction to Gibbs Free Energy=	0.210936
Sum of electronic and zero-point Energies=	-405.899577
Sum of electronic and thermal Energies=	-405.886848
Sum of electronic and thermal Enthalpies=	-405.885904
Sum of electronic and thermal Free Energies=	-405.940809

TS_13

Zero-point correction=	0.250629
(Hartree/Particle)	
Thermal correction to Energy=	0.262062
Thermal correction to Enthalpy=	0.263006
Thermal correction to Gibbs Free Energy=	0.214254
Sum of electronic and zero-point Energies=	-405.909339
Sum of electronic and thermal Energies=	-405.897906
Sum of electronic and thermal Enthalpies=	-405.896962
Sum of electronic and thermal Free Energies=	-405.945714

TS_14

Zero-point correction=	0.256992
(Hartree/Particle)	
Thermal correction to Energy=	0.267829
Thermal correction to Enthalpy=	0.268773
Thermal correction to Gibbs Free Energy=	0.221719
Sum of electronic and zero-point Energies=	-405.949928
Sum of electronic and thermal Energies=	-405.939091
Sum of electronic and thermal Enthalpies=	-405.938146
Sum of electronic and thermal Free Energies=	-405.985200