Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Dual Roles of Electronic Effect on the Selectivity: Pincer Nickel Electrocatalyzed CO_2 Reduction

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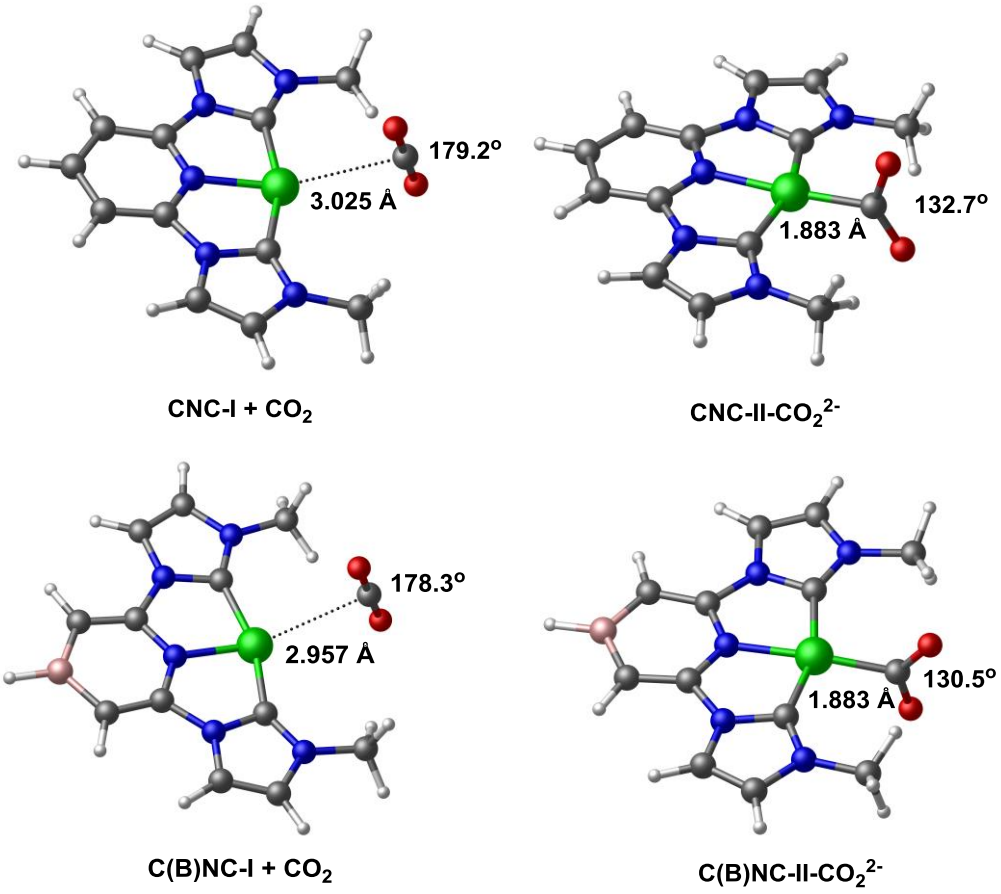

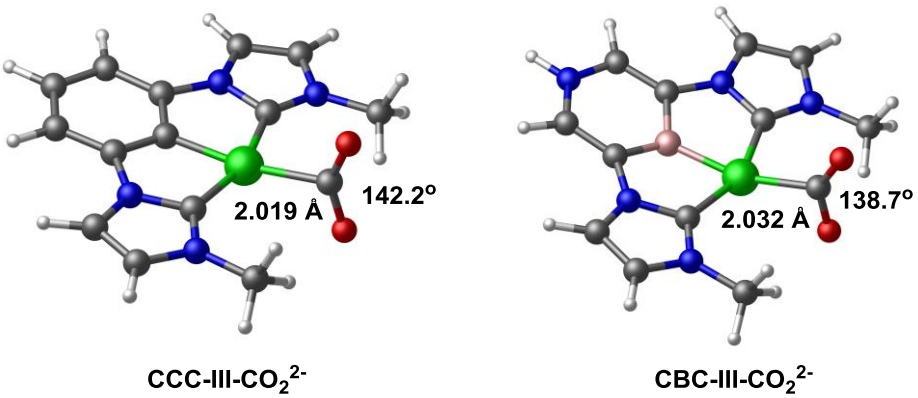

Figure S1. Calculated structures of the intermediates generated after the CO_2 coordination step.

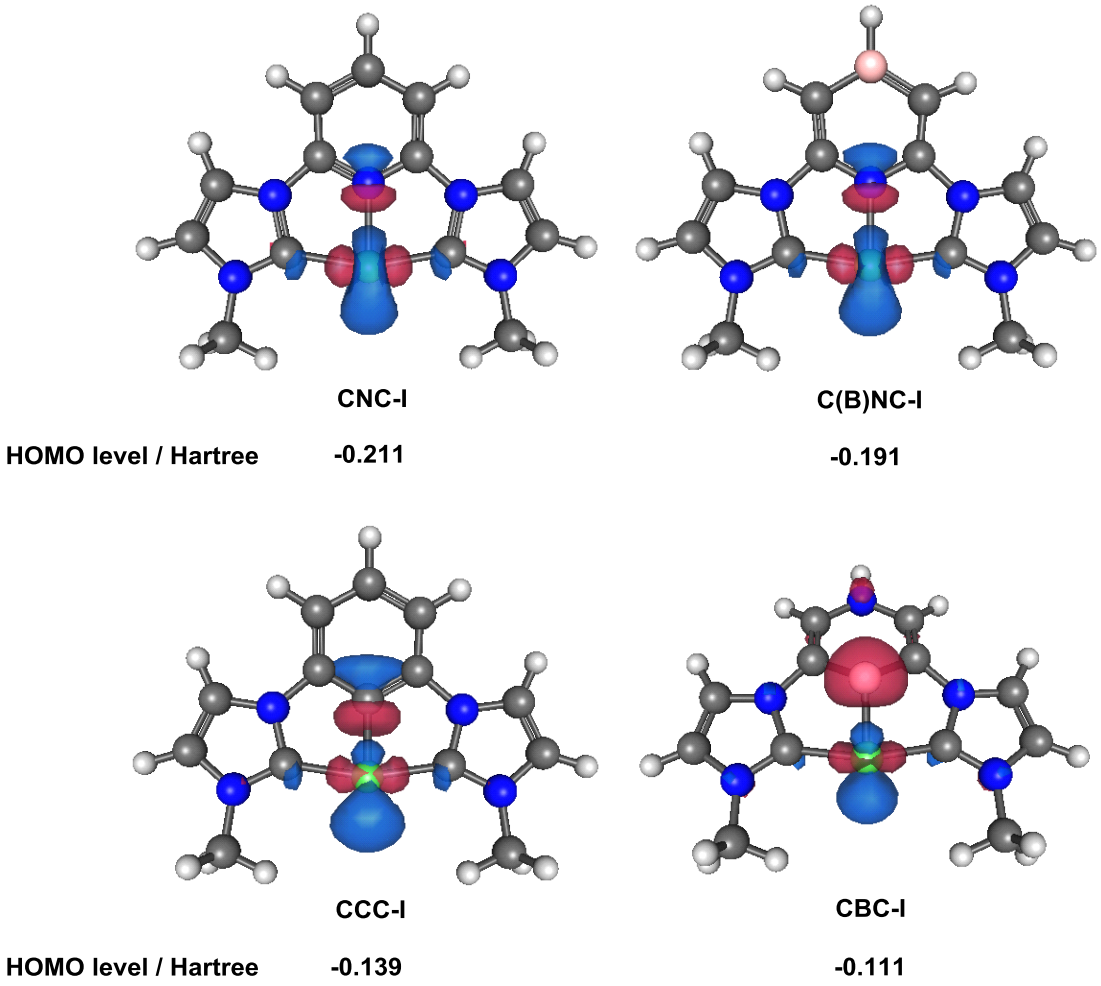

Figure S2. The HOMO of **CNC-I**, **C(B)NC-I**, **CCC-I** and **CBC-I**.

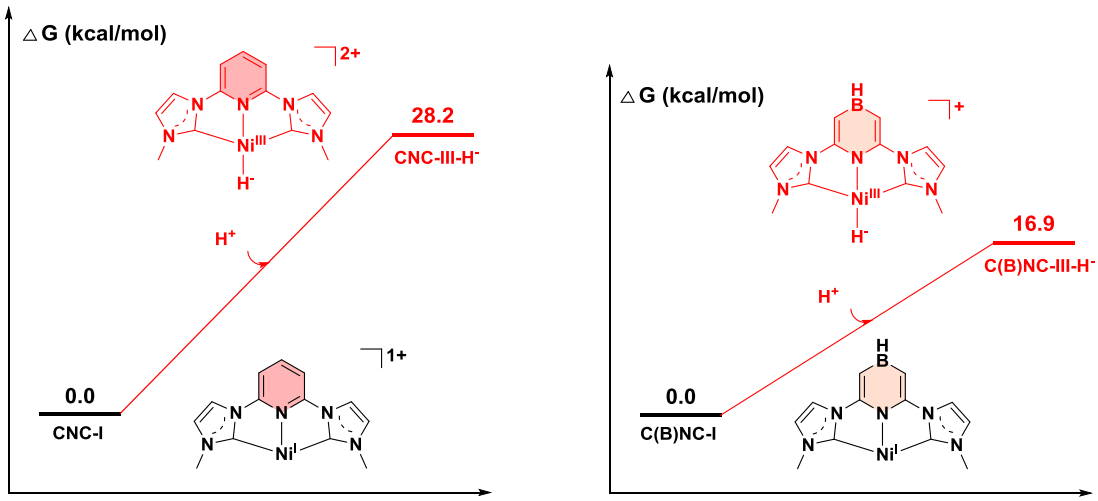

Figure S3. The highly endothermic protonation step of **CNC-I** and **C(B)NC-I**.

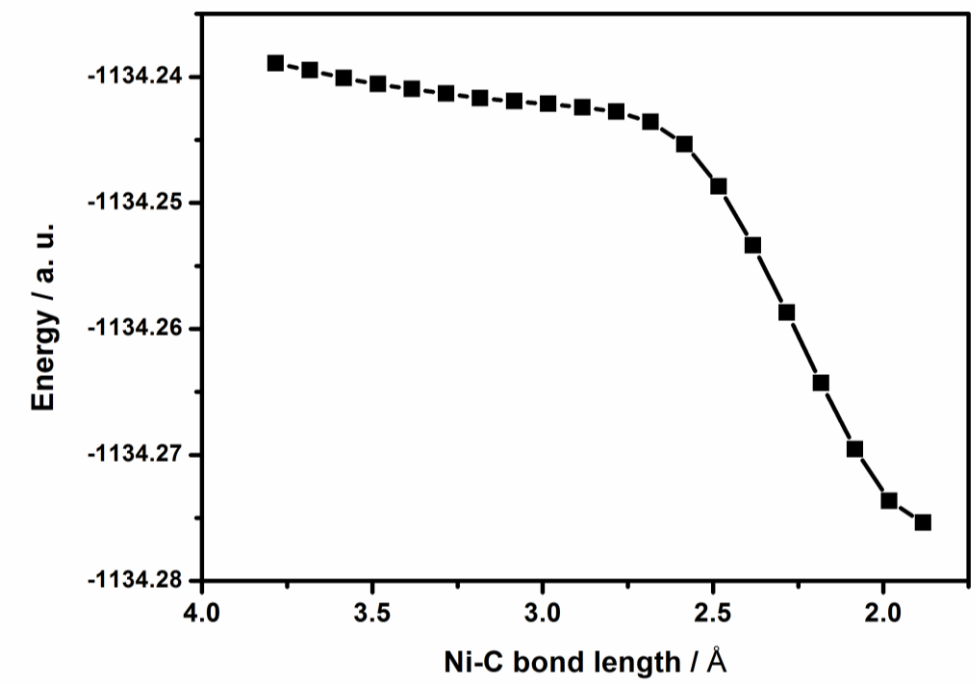

Figure S4. Relax scan of Ni-C distance for the CO_2 coordination step of **CNC-0**.

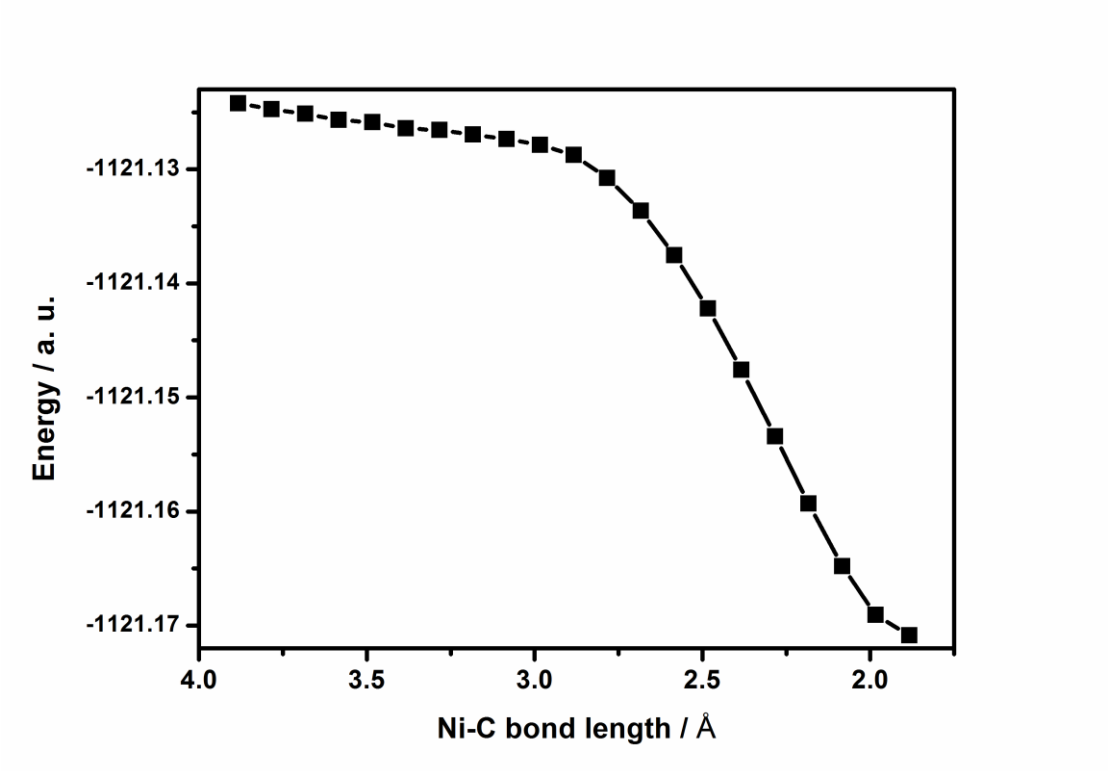

Figure S5. Relax scan of Ni-C distance for CO_2 coordination step of **C(B)NC-0**.

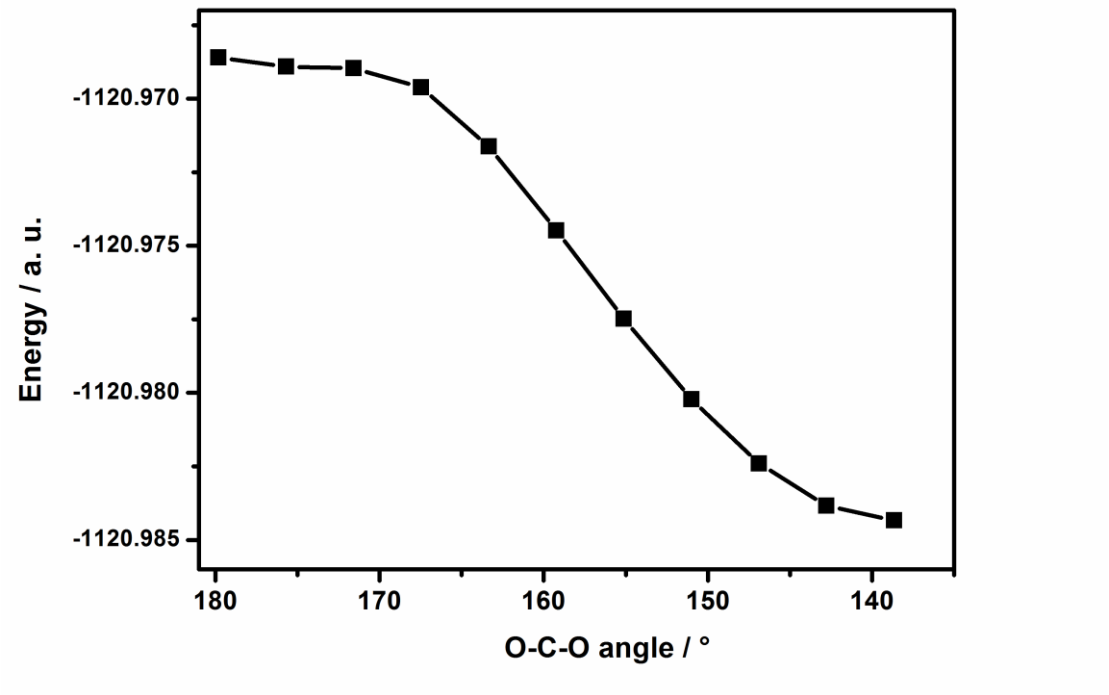

Figure S6. Relax scan of the O-C-O angle for the CO_2 coordination step of **CBC-I**.

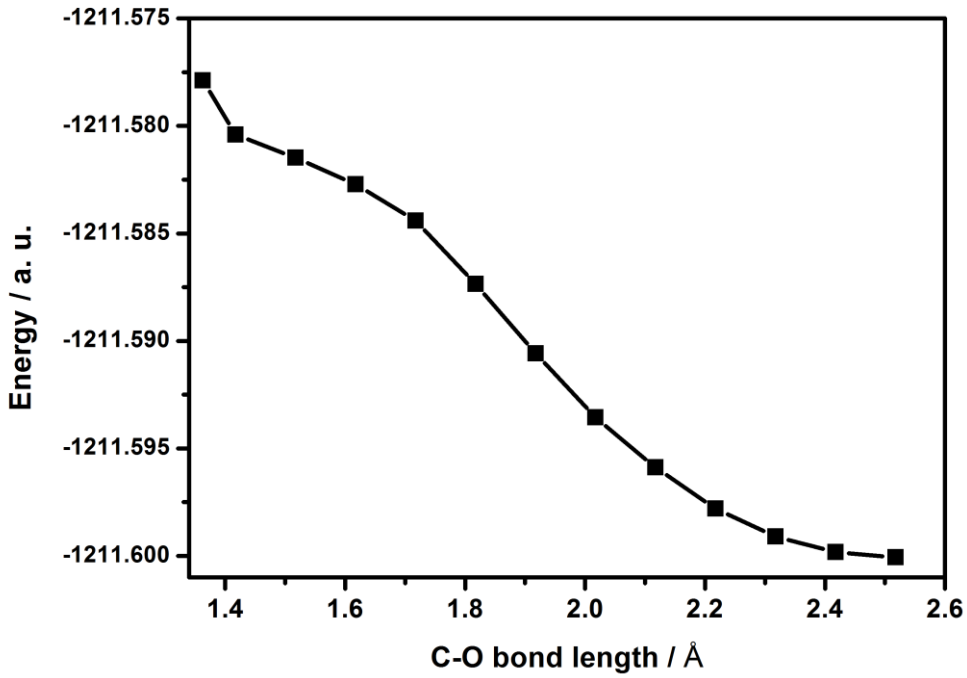

Figure S7 Relax scan of C-O distance for the C-O cleavage step of **CNC-II-COOH**$^-$ assisted by H_3O^+.

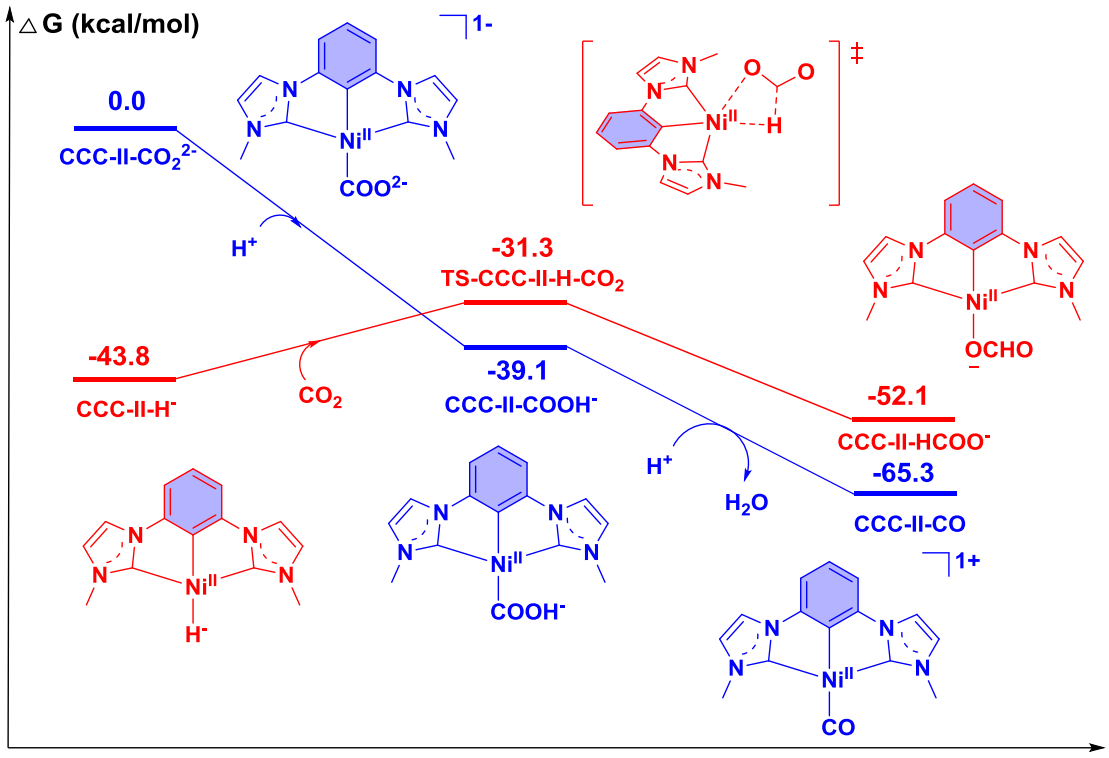

Figure S8. Free-energy profile for the pathway of CO_2 reduced by **CCC-II-CO_2^{2-}** and **CCC-II-H^-**. Free energies at the M06 / LANL2TZ(f) (6-311+G(2d,p) (SMD) // M06 / LANL2DZ (6-31G(d,p) (SMD) level of theory are given in kcal/mol. The free energy of **CCC-II-CO_2^{2-}** is set as 0.

.

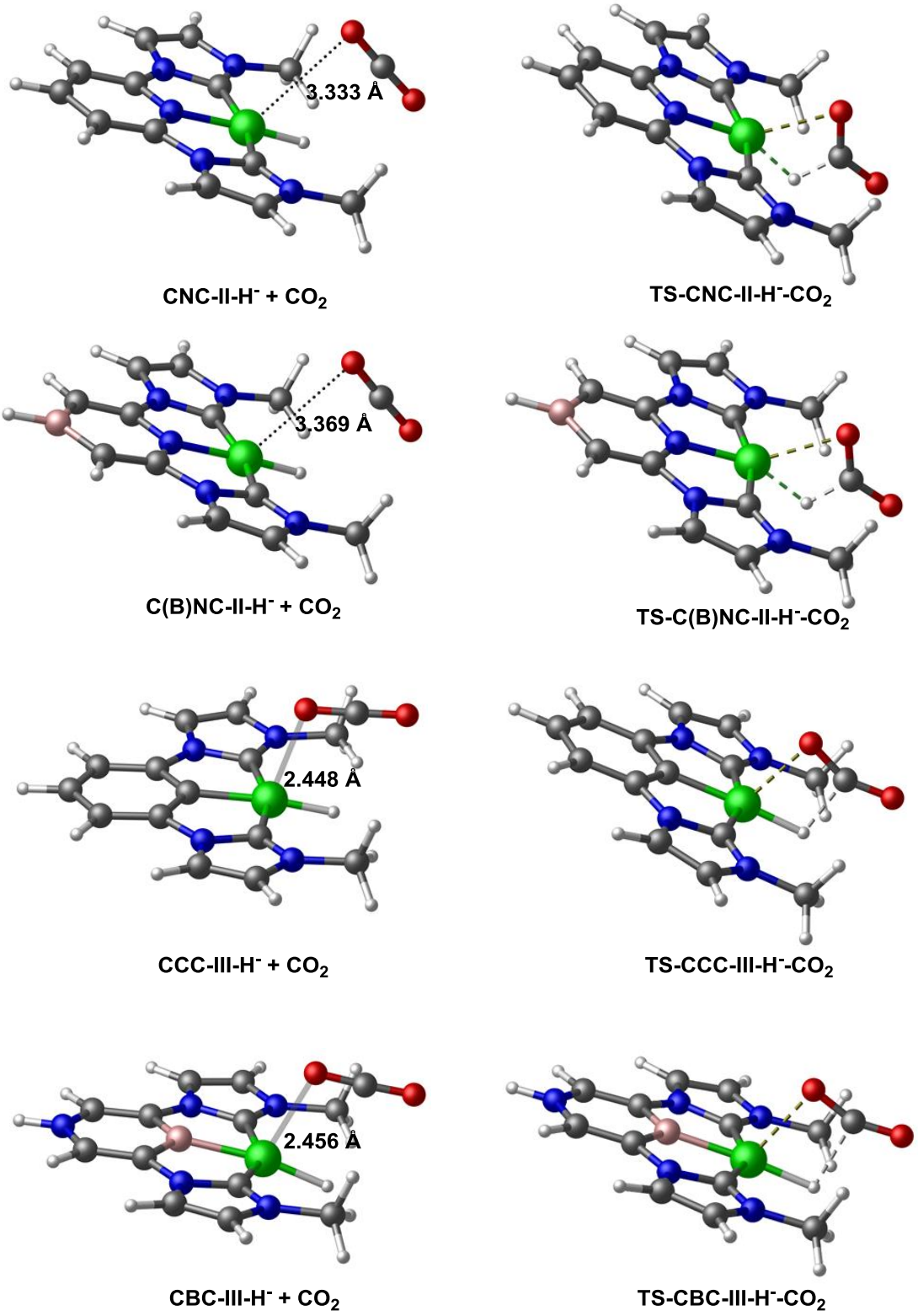

Figure S9. Calculated structures of the intermediates and transitions states in Figure 9.

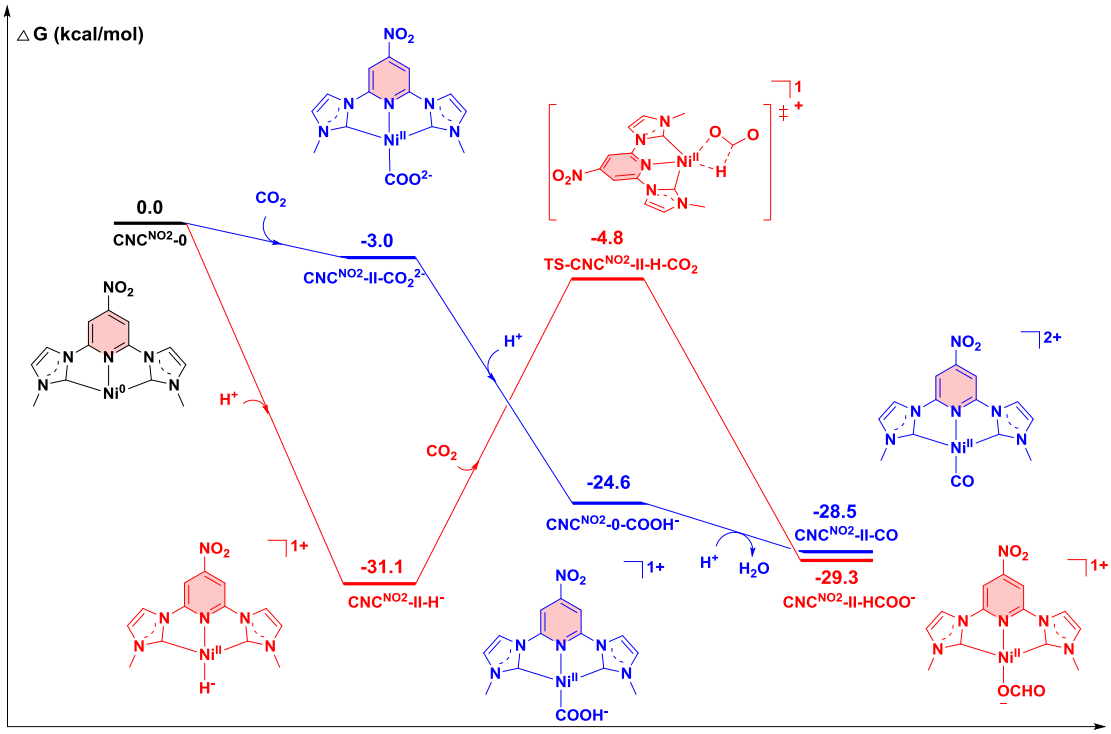

Figure S10. Free-energy profile for the pathway of CO_2 reduced by **CNC^{NO2}-0**

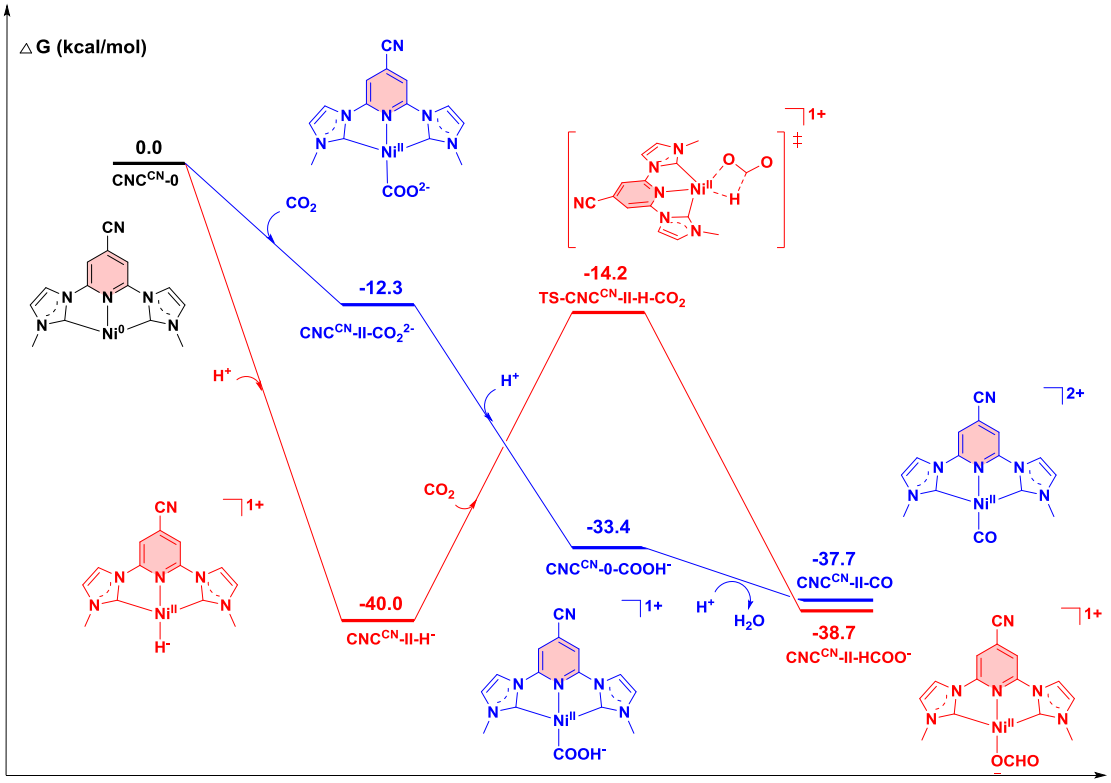

Figure S11. Free-energy profile for the pathway of CO_2 reduced by **CNC^{CN}-0**

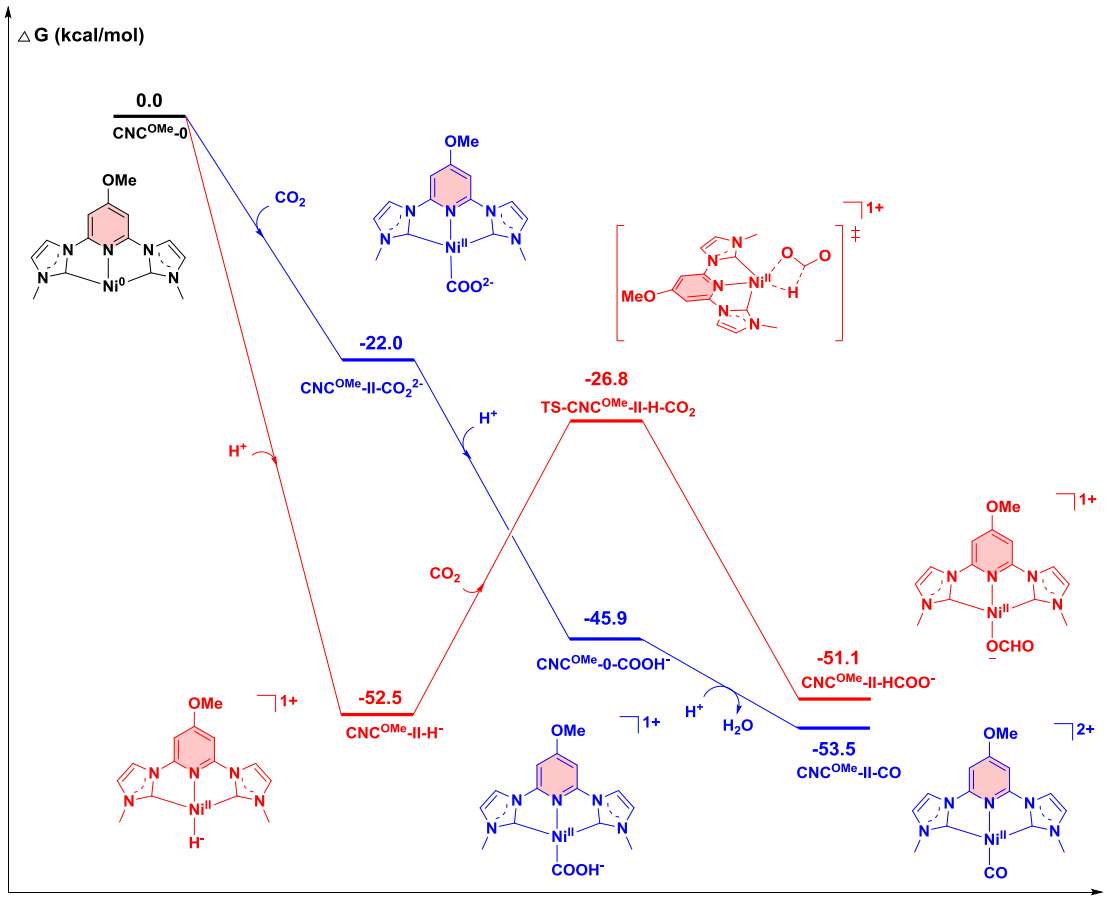

Figure S12. Free-energy profile for the pathway of CO_2 reduced by **CNC^{OMe}-0**

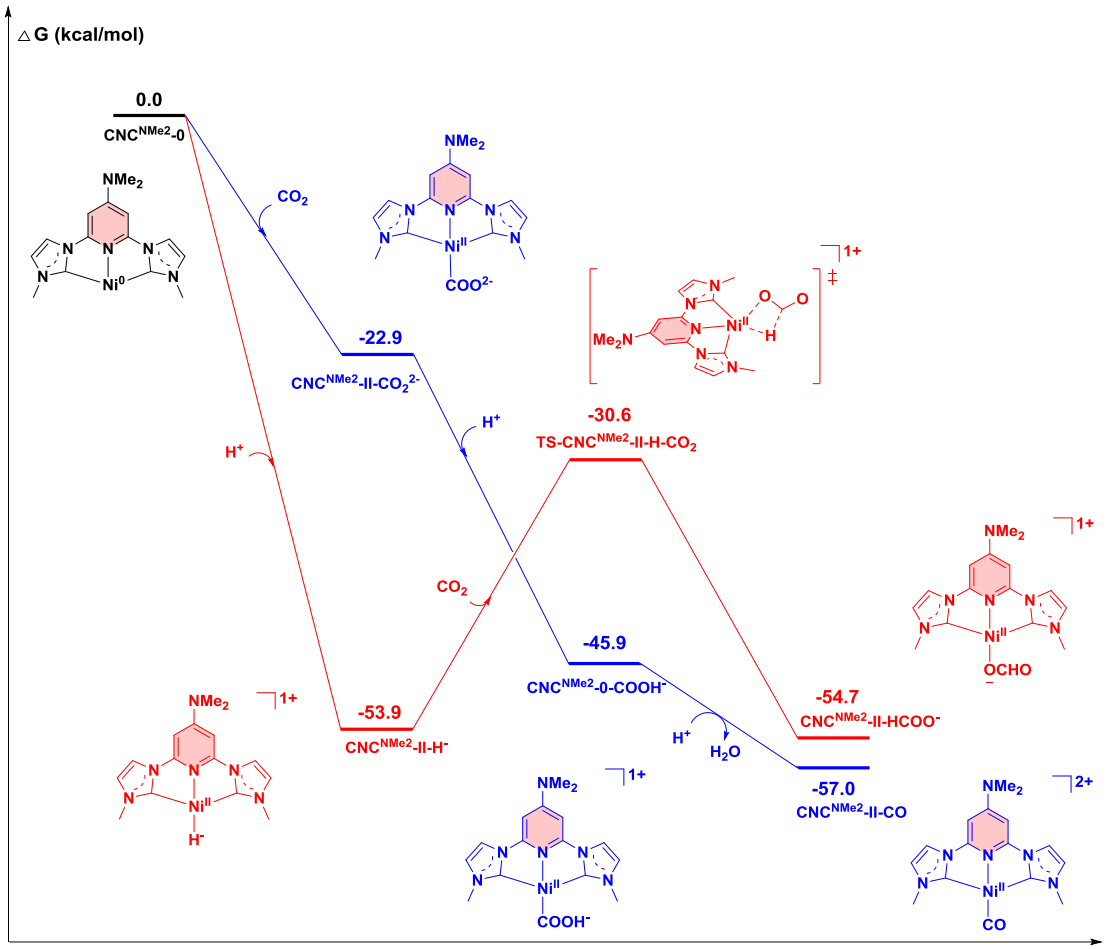

Figure S13. Free-energy profile for the pathway of CO_2 reduced by **CNC^{NMe2}-0**

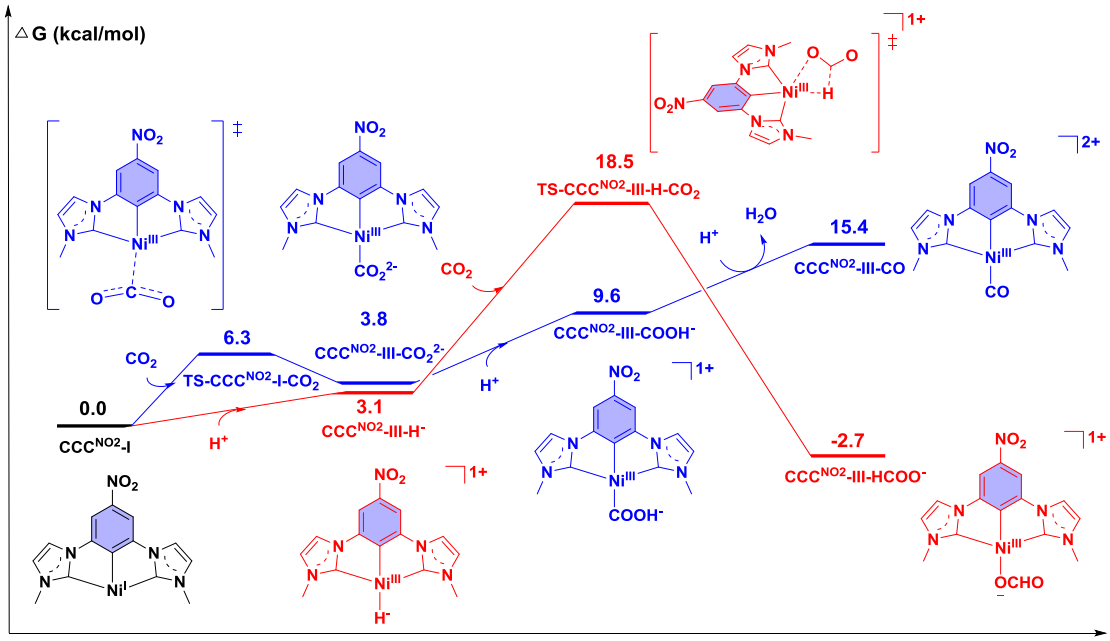

Figure S14. Free-energy profile for the pathway of CO_2 reduced by **CCC^{NO2}-I**

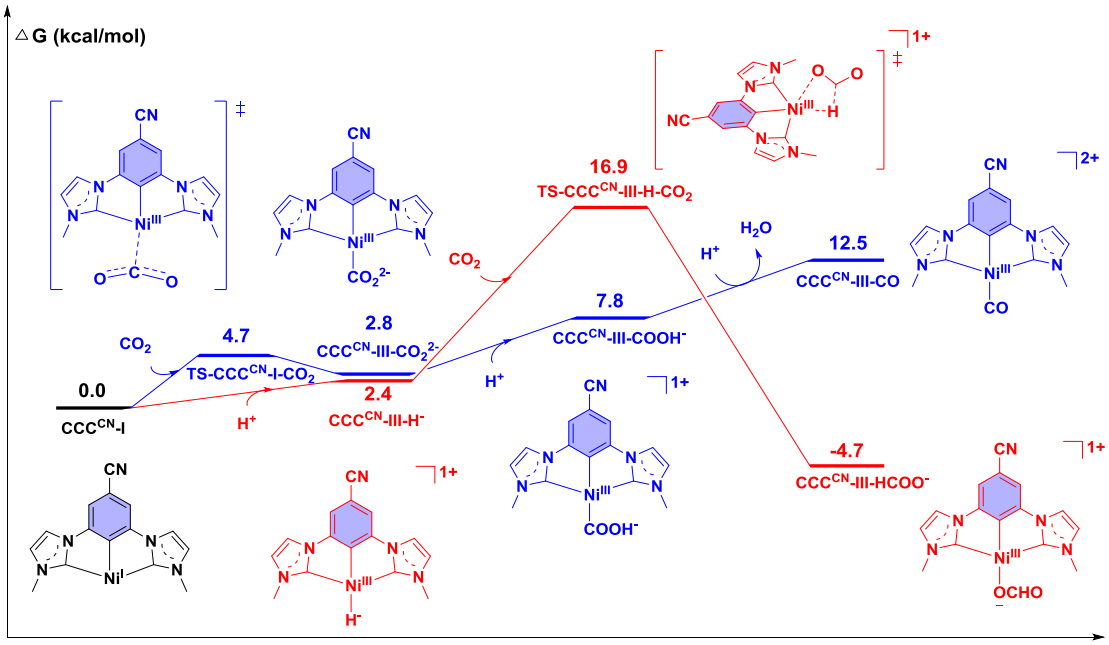

Figure S15. Free-energy profile for the pathway of CO_2 reduced by **CCC^{CN}-I**

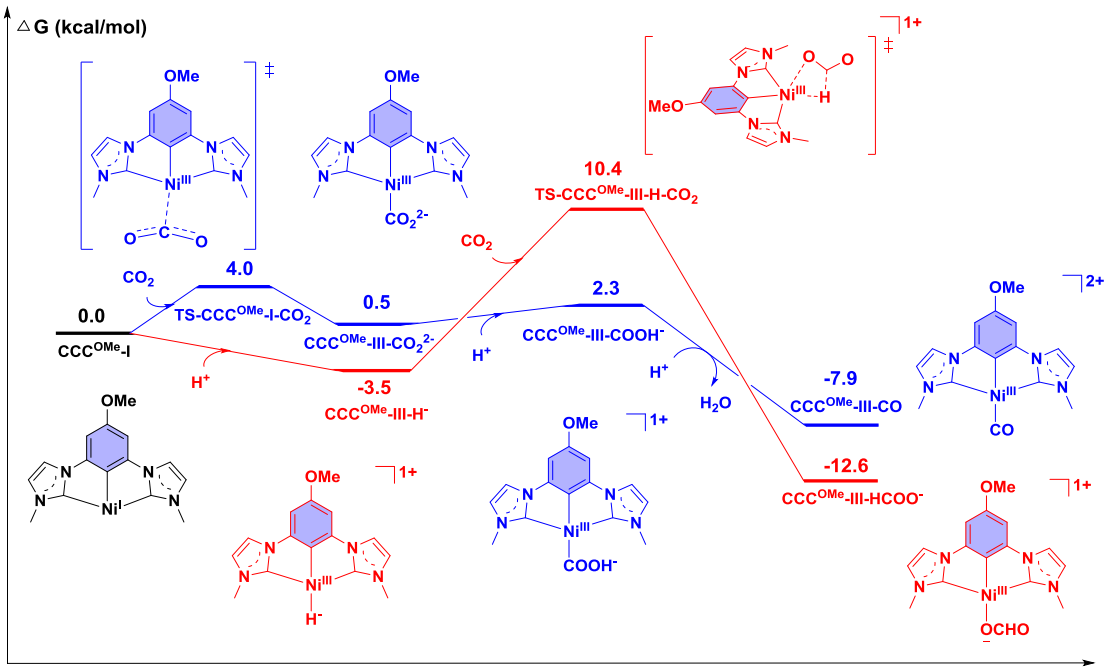

Figure S16. Free-energy profile for the pathway of CO_2 reduced by **CCC^{OMe}-I**

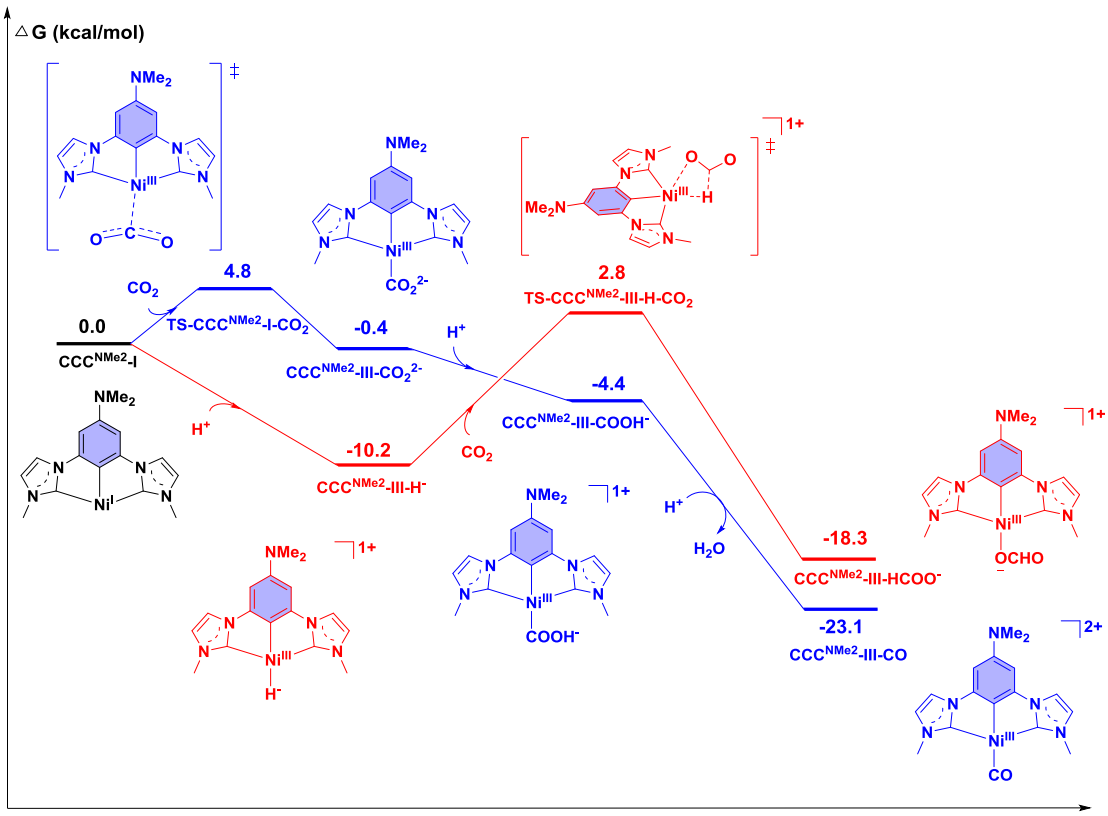

Figure S17. Free-energy profile for the pathway of CO_2 reduced by **CCC^{NMe2}-I**

Optimized coordinates (xyz) optimized at the BP86/BSI level of theory

CCC-II-CO

1 1

28 0.000047 -0.725319 -0.000394

7 2.276032 0.939020 -0.002713

7 -2.275975 0.939048 -0.002624

7 -3.079233 -1.047892 -0.028152

7 3.079190 -1.047980 -0.027917

6 1.913907 -0.377454 -0.009672

6 1.192156 1.850086 0.005836

6 -1.192095 1.850094 0.005880

6 -1.913896 -0.377446 -0.009862

6 -4.151034 -0.169064 -0.031142

1 -5.172090 -0.523222 -0.045124

6 -3.642691 1.090259 -0.014752

1 -4.128018 2.055622 -0.012395

6 -3.222295 -2.496632 -0.038841

1 -2.724330 -2.918382 -0.915570

1 -4.284699 -2.739666 -0.087268

1 -2.804913 -2.923919 0.876657

6 -1.225564 3.239333 0.023933

1 -2.163659 3.788847 0.032289

6 0.000040 3.913201 0.032209

1 0.000044 5.000260 0.046718

6 1.225640 3.239323 0.023842

1 2.163740 3.788830 0.032134

6 3.642755 1.090153 -0.015319

1 4.128135 2.055489 -0.013351

6 4.151036 -0.169213 -0.031136

1 5.172075 -0.523427 -0.044958

6 3.222076 -2.496741 -0.038502

1 2.803991 -2.923919 0.876716

1 4.284486 -2.739912 -0.086054

1 2.724641 -2.918487 -0.915558

6 -0.000050 -2.540586 0.058208

8 -0.000106 -3.680480 0.119488

6 0.000023 1.154566 -0.003895

CCC-II-COOH$^-$

0 1

28 0.001276 -0.568481 0.031101

7 -2.278151 1.080966 0.003795

7 2.265418 1.101277 0.011583

7 3.093184 -0.875891 0.004710

7 -3.089214 -0.902947 0.024300

6 -1.910824 -0.245304 0.021912

6 -1.200356 2.010422 0.001458

6 1.179510 2.021266 0.005961

6 1.909213 -0.228157 0.011205

6 4.156606 0.014092 0.006985

1 5.182638 -0.326549 0.002153

6 3.631640 1.266111 0.008516

1 4.107654 2.236496 0.002472

6 3.255820 -2.321046 0.033371

1 3.151767 -2.697816 1.055211

1 4.250519 -2.571030 -0.341958

1 2.500391 -2.782945 -0.605355

6 1.211618 3.412255 -0.025636

1 2.144575 3.972103 -0.040909

6 -0.019643 4.080608 -0.040414

1 -0.024513 5.168114 -0.064608

6 -1.244839 3.401038 -0.030351

1 -2.182646 3.952602 -0.048737

6 -3.645712 1.234111 -0.010119

1 -4.129821 2.200458 -0.019563

6 -4.160127 -0.022248 0.000826

1 -5.183268 -0.371559 -0.000005

6 -3.239681 -2.349589 0.001469

1 -3.160895 -2.725262 -1.023362

1 -4.221341 -2.608835 0.404096

1 -2.461472 -2.804671 0.616864

6 0.011166 -2.466844 0.077450

8 -0.044511 -3.192910 1.063752

8 0.094952 -3.089054 -1.149165

6 -0.007328 1.319319 0.024557

1 0.086115 -4.047979 -0.957678

CCC-II-CO_2^{2-}

-1 1

28 0.000033 -0.616676 0.094780

7 2.267663 1.053798 0.036266

7 -2.267430 1.054060 0.036605

7 -3.109552 -0.915204 -0.104015

7 3.109510 -0.915630 -0.103942

6 1.911930 -0.282595 -0.038516

6 1.187334 1.981709 0.104022

6 -1.186977 1.981833 0.104243

6 -1.911894 -0.282396 -0.038169
6 -4.169031 -0.019375 -0.076223
1 -5.198192 -0.349433 -0.120001
6 -3.635375 1.225483 0.004490
1 -4.107166 2.197600 0.043379
6 -3.272849 -2.355593 -0.183733
1 -2.367686 -2.787496 -0.621151
1 -4.138459 -2.588118 -0.810559
1 -3.429101 -2.783522 0.812231
6 -1.226886 3.361273 -0.086739
1 -2.160916 3.907374 -0.213054
6 0.000275 4.037563 -0.144210
1 0.000318 5.116503 -0.286382
6 1.227368 3.361142 -0.086983
1 2.161439 3.907133 -0.213476
6 3.635647 1.224979 0.004602
1 4.107592 2.197017 0.043563
6 4.169121 -0.019979 -0.075844
1 5.198246 -0.350197 -0.119259
6 3.272489 -2.356078 -0.183512
1 3.428324 -2.783948 0.812556
1 4.138224 -2.588900 -0.810054
1 2.367328 -2.787790 -0.621148
6 -0.000355 -2.526161 0.025157
8 0.000114 -3.341554 -0.922186
8 -0.001112 -2.749181 1.265596
6 0.000163 1.292761 0.279390

CCC-III-CO

2 2

28 -0.012037 -0.712341 -0.006591
7 -2.255322 0.986612 0.005789
7 2.298247 0.916674 0.008473
7 3.029428 -1.112788 0.044949
7 -3.096448 -0.984390 0.042005
6 -1.922684 -0.340627 0.012232
6 -1.160437 1.865937 -0.007633
6 1.265929 1.825826 -0.010152
6 1.889005 -0.428783 0.019561
6 4.124091 -0.255583 0.049052
1 5.136037 -0.636942 0.070076
6 3.659614 1.025538 0.025248
1 4.180132 1.972309 0.022269
6 3.146773 -2.569319 0.061601
1 2.623147 -2.969453 0.932355
1 4.203742 -2.826277 0.130767
1 2.737993 -2.980271 -0.864342
6 1.334034 3.218536 -0.038261
1 2.282607 3.745736 -0.049978
6 0.128278 3.896861 -0.049692
6 -1.139244 3.240258 -0.034893
1 -2.052325 3.829405 -0.048029
6 -3.619467 1.168057 0.028952
1 -4.083129 2.143852 0.029705
6 -4.149430 -0.080839 0.052168
1 -5.177038 -0.414696 0.076266
6 -3.274604 -2.431194 0.058491
1 -2.893904 -2.865638 -0.869227
1 -4.340814 -2.646856 0.136994
1 -2.763762 -2.860020 0.923989

6 -0.073971 -2.552005 -0.093909

8 -0.111574 -3.685475 -0.174078

6 0.027229 1.136062 0.002222

1 0.134912 4.983114 -0.072101

CCC-III-COOH$^-$

1 2

28 -0.000046 -0.586171 -0.317781

7 -2.280058 1.032686 -0.067331

7 2.279860 1.033097 -0.068626

7 3.081992 -0.946485 -0.274533

7 -3.082044 -0.946796 -0.274770

6 -1.922910 -0.276522 -0.236855

6 -1.203489 1.949383 0.017519

6 1.203171 1.949624 0.016699

6 1.922826 -0.276215 -0.237560

6 4.154928 -0.079668 -0.127897

1 5.175013 -0.436972 -0.138487

6 3.648106 1.172932 0.002892

1 4.134451 2.129766 0.128279

6 3.214674 -2.390480 -0.400087

1 3.298280 -2.846795 0.591003

1 4.111263 -2.616683 -0.980849

1 2.337374 -2.786714 -0.913551

6 1.230266 3.327452 0.196277

1 2.164796 3.877306 0.275250

6 -0.000268 3.990200 0.278798

1 -0.000329 5.067994 0.420488

6 -1.230726 3.327200 0.197147

1 -2.165309 3.876869 0.276794

6 -3.648342 1.172452 0.003566

1 -4.134772 2.129196 0.129314

6 -4.155068 -0.080092 -0.128102

1 -5.175130 -0.437446 -0.139242

6 -3.214612 -2.390768 -0.400825

1 -2.337211 -2.786794 -0.914288

1 -4.111084 -2.616813 -0.981824

1 -3.298220 -2.847416 0.590102

6 0.000468 -2.166586 0.767788

8 0.001577 -2.182638 1.969528

8 -0.000318 -3.259511 -0.012500

6 -0.000129 1.286145 -0.093977

1 0.000471 -4.053373 0.563163

CCC-III-CO_2^{2-}

0 2

28 0.000020 -0.600568 -0.109647

7 2.276125 1.046088 -0.030185

7 -2.276140 1.046035 -0.029690

7 -3.109274 -0.926869 -0.103235

7 3.109254 -0.926840 -0.103137

6 1.925183 -0.282644 -0.083228

6 1.194410 1.969094 -0.005515

6 -1.194437 1.969065 -0.005230

6 -1.925194 -0.282694 -0.082736

6 -4.171174 -0.035965 -0.054281

1 -5.198007 -0.374332 -0.062723

6 -3.643038 1.213358 -0.008892

1 -4.115807 2.184687 0.026132

6 -3.271923 -2.371904 -0.118657

1 -2.421421 -2.821941 -0.634233
1 -4.192354 -2.622525 -0.651264
1 -3.330319 -2.760315 0.902932
6 -1.228882 3.356255 0.103687
1 -2.163825 3.910048 0.159493
6 -0.000021 4.027442 0.147818
1 -0.000022 5.111815 0.231943
6 1.228849 3.356285 0.103367
1 2.163791 3.910106 0.158918
6 3.643018 1.213393 -0.008916
1 4.115794 2.184715 0.026150
6 4.171152 -0.035948 -0.053928
1 5.197982 -0.374333 -0.061901
6 3.271851 -2.371885 -0.118544
1 3.329708 -2.760334 0.903068
1 4.192538 -2.622519 -0.650687
1 2.421566 -2.821859 -0.634524
6 0.000080 -2.578813 0.292789
8 0.000035 -3.063367 -0.836637
8 0.000079 -2.884576 1.467828
6 -0.000016 1.286183 -0.079236

CCC-III-HCOO$^-$

1 2
28 0.000003 -0.649357 -0.211165
7 -2.289067 1.013288 -0.064507
7 2.288863 1.013551 -0.065183
7 3.093303 -0.969953 -0.225960
7 -3.093280 -0.970254 -0.225968
6 -1.939371 -0.295719 -0.200358
6 -1.203455 1.913208 0.008356
6 1.203198 1.913337 0.007984
6 1.939338 -0.295504 -0.201119
6 4.164565 -0.095972 -0.103752
1 5.185015 -0.452502 -0.108496
6 3.657452 1.159303 -0.002505
1 4.142211 2.119584 0.099346
6 3.229027 -2.417950 -0.313847
1 3.343312 -2.841566 0.688587
1 4.110643 -2.655987 -0.912335
1 2.336359 -2.829514 -0.786426
6 1.226235 3.297513 0.129603
1 2.163956 3.845121 0.178092
6 -0.000237 3.965558 0.188341
1 -0.000258 5.048183 0.283550
6 -1.226640 3.297403 0.129976
1 -2.164422 3.844880 0.178727
6 -3.657688 1.158957 -0.002683
1 -4.142571 2.119198 0.098953
6 -4.164655 -0.096368 -0.104206
1 -5.185074 -0.452979 -0.109390
6 -3.228731 -2.418298 -0.313643
1 -2.337149 -2.829556 -0.788533
1 -4.111835 -2.656490 -0.909858
1 -3.340328 -2.842060 0.689033
6 0.000379 -2.778094 0.876962
8 0.000764 -1.755657 1.606764
8 -0.000144 -2.661289 -0.385361
6 -0.000104 1.239051 -0.052060
1 0.000499 -3.783731 1.329160

CCC-III-H$^-$

1 2

28 -0.000003 -1.007731 -0.000317

7 -2.281299 0.660888 0.000148

7 2.281297 0.660884 0.000011

7 3.095062 -1.329258 -0.000229

7 -3.095057 -1.329259 -0.000030

6 -1.934491 -0.662929 -0.000095

6 -1.199822 1.584136 0.000273

6 1.199822 1.584132 0.000200

6 1.934492 -0.662934 -0.000227

6 4.162681 -0.445360 -0.000003

1 5.185120 -0.796078 0.000021

6 3.648485 0.812132 0.000119

1 4.131562 1.778826 0.000302

6 3.247915 -2.776000 -0.000406

1 2.254892 -3.229365 -0.000751

1 3.796864 -3.086532 0.892285

1 3.797370 -3.086257 -0.892880

6 1.230205 2.974417 0.000362

1 2.164012 3.531269 0.000384

6 0.000002 3.642999 0.000461

1 0.000003 4.730210 0.000574

6 -1.230203 2.974420 0.000435

1 -2.164008 3.531274 0.000509

6 -3.648487 0.812131 0.000320

1 -4.131568 1.778823 0.000520

6 -4.162679 -0.445363 0.000199

1 -5.185116 -0.796084 0.000251

6 -3.247907 -2.776001 -0.000186

1 -3.797370 -3.086268 -0.892652

1 -3.796848 -3.086525 0.892514

1 -2.254883 -3.229363 -0.000538

6 -0.000001 0.911103 0.000170

1 -0.000037 -2.541544 -0.000693

CCC-I

0 2

28 -0.000070 -1.014422 0.070042

7 2.275043 0.618968 0.069814

7 -2.275059 0.618962 0.070210

7 -3.155378 -1.332563 -0.049378

7 3.155486 -1.332535 -0.049140

6 1.947758 -0.723430 -0.002946

6 1.189588 1.553043 0.122353

6 -1.189593 1.553069 0.122616

6 -1.947670 -0.723398 -0.003034

6 -4.199294 -0.419904 -0.017766

1 -5.234500 -0.732051 -0.045595

6 -3.639450 0.814144 0.051651

1 -4.091556 1.795231 0.098604

6 -3.343847 -2.767675 -0.138610

1 -2.360176 -3.239471 -0.209917

1 -3.932148 -3.018306 -1.026509

1 -3.861143 -3.141354 0.750396

6 -1.229430 2.924969 -0.117438

1 -2.161562 3.468403 -0.267553

6 -0.000029 3.596053 -0.197005

1 -0.000045 4.669209 -0.377127

6 1.229365 2.924945 -0.117741
1 2.161462 3.468362 -0.268110
6 3.639432 0.814229 0.051146
1 4.091468 1.795369 0.097679
6 4.199355 -0.419793 -0.017921
1 5.234573 -0.731884 -0.045855
6 3.343972 -2.767682 -0.137812
1 3.860552 -3.141159 0.751705
1 3.933020 -3.018518 -1.025147
1 2.360353 -3.239505 -0.209678
6 0.000012 0.884707 0.323405

CNC-II-CO

2 1
28 -0.000009 -0.708821 0.002120
7 2.224678 0.907928 -0.005173
7 -2.224869 0.907670 -0.005710
7 -3.075060 -1.060819 -0.029016
7 3.075162 -1.060414 -0.029155
6 1.904592 -0.423230 -0.009774
6 1.164482 1.815714 0.003945
6 -1.164772 1.815584 0.003631
6 -1.904609 -0.423433 -0.010027
6 -4.125965 -0.151893 -0.035314
1 -5.154501 -0.482966 -0.050705
6 -3.594773 1.093425 -0.020460
1 -4.052038 2.072328 -0.020958
6 -3.252057 -2.509497 -0.040847
1 -2.771415 -2.934682 -0.925149
1 -4.319980 -2.726034 -0.078041
1 -2.833262 -2.940734 0.871712
6 -1.219680 3.195380 0.028120
1 -2.170339 3.717658 0.039884
6 -0.000267 3.872461 0.039619
1 -0.000334 4.958457 0.060400
6 1.219223 3.195520 0.028459
1 2.169823 3.717903 0.040491
6 3.594545 1.093903 -0.020288
1 4.051655 2.072878 -0.020589
6 4.125923 -0.151323 -0.035568
1 5.154505 -0.482247 -0.051148
6 3.252445 -2.509050 -0.041233
1 2.833969 -2.940467 0.871389
1 4.320404 -2.725365 -0.078634
1 2.771670 -2.934224 -0.925461
6 -0.000017 -2.494382 0.068931
8 0.000875 -3.629060 0.126288
7 -0.000104 1.161620 -0.010664

CNC-II-COOH$^-$

1 1
28 0.000004 -0.579556 0.020734
7 -2.220032 1.053441 0.005222
7 2.219726 1.053757 0.005158
7 3.092222 -0.901489 -0.006604
7 -3.092102 -0.902028 -0.006673
6 -1.902206 -0.289858 -0.001434
6 -1.162366 1.973682 0.001003
6 1.161922 1.973842 0.000985
6 1.902172 -0.289604 -0.001714

6 4.136064 0.017189 0.002411

1 5.168918 -0.301084 -0.000659

6 3.589110 1.254424 0.007211

1 4.036965 2.237842 0.007115

6 3.287472 -2.345252 0.016240

1 3.208507 -2.720471 1.040119

1 4.280163 -2.570341 -0.377893

1 2.533500 -2.821150 -0.613543

6 1.221720 3.357292 -0.018583

1 2.169295 3.885587 -0.028861

6 -0.000350 4.031912 -0.026207

1 -0.000429 5.118360 -0.041587

6 -1.222328 3.357122 -0.018588

1 -2.169957 3.885311 -0.028898

6 -3.589484 1.253781 0.006875

1 -4.037555 2.237103 0.006508

6 -4.136159 0.016419 0.002050

1 -5.168944 -0.302073 -0.001299

6 -3.286728 -2.345859 0.016701

1 -2.533001 -2.821639 -0.613493

1 -4.279591 -2.571536 -0.376683

1 -3.206884 -2.720732 1.040631

6 0.000258 -2.426208 0.094076

8 0.000165 -3.099110 1.105316

8 0.000598 -3.025224 -1.129296

1 0.000750 -3.989796 -0.967389

7 -0.000177 1.331114 0.014479

CNC-II-CO_2^{2-}

0 1

28 0.000072 -0.660855 0.038655

7 2.217341 1.029038 0.018531

7 -0.000118 1.321418 0.099508

7 -2.217516 1.028803 0.018136

7 -3.117231 -0.909230 -0.109310

7 3.117246 -0.908891 -0.109375

6 1.908223 -0.324112 -0.045070

6 1.159704 1.955145 0.045341

6 -1.159981 1.955030 0.045107

6 -1.908260 -0.324302 -0.045451

6 -4.150857 0.020991 -0.083794

1 -5.188724 -0.279122 -0.127443

6 -3.585784 1.247184 -0.008511

1 -4.021974 2.235537 0.025061

6 -3.322004 -2.347695 -0.177721

1 -2.424437 -2.807409 -0.599514

1 -4.182513 -2.559241 -0.817422

1 -3.507078 -2.754194 0.821520

6 -1.223658 3.340858 -0.008081

1 -2.169098 3.872647 -0.047043

6 -0.000238 4.015051 -0.021727

1 -0.000289 5.101157 -0.063129

6 1.223246 3.340982 -0.007801

1 2.168644 3.872868 -0.046525

6 3.585571 1.247580 -0.008590

1 4.021664 2.235975 0.024961

6 4.150761 0.021455 -0.084157

1 5.188650 -0.278531 -0.128162

6 3.322098 -2.347350 -0.177840

1 3.505429 -2.754147 0.821606

1 4.183711 -2.558695 -0.816102
1 2.425214 -2.806962 -0.601198
6 0.000329 -2.541136 0.139931
8 0.000207 -3.234873 -0.889991
8 0.000523 -2.827878 1.349841

CNC-II-HCOO$^-$

1 1
28 0.000027 -0.583572 -0.225481
7 -2.228429 1.027488 -0.040742
7 2.228358 1.027683 -0.040787
7 3.081472 -0.927076 -0.228945
7 -3.081513 -0.927287 -0.228878
6 -1.905263 -0.299922 -0.185590
6 -1.164424 1.928616 0.042361
6 1.164301 1.928748 0.042326
6 1.905205 -0.299731 -0.185601
6 4.134395 -0.024760 -0.107752
1 5.163811 -0.353991 -0.123003
6 3.600594 1.212986 0.009090
1 4.058102 2.186098 0.114876
6 3.251754 -2.369771 -0.343298
1 3.388220 -2.808555 0.649602
1 4.130949 -2.577040 -0.956871
1 2.360885 -2.789204 -0.812648
6 1.218794 3.302722 0.195441
1 2.168989 3.822735 0.257891
6 -0.000177 3.976264 0.266864
1 -0.000222 5.055957 0.386218
6 -1.219067 3.302601 0.195474
1 -2.169324 3.822498 0.257967
6 -3.600671 1.212774 0.009196
1 -4.058157 2.185902 0.114937
6 -4.134441 -0.024988 -0.107614
1 -5.163850 -0.354246 -0.122732
6 -3.251859 -2.369995 -0.343177
1 -2.361187 -2.789440 -0.812896
1 -4.131335 -2.577223 -0.956375
1 -3.387883 -2.808770 0.649802
6 0.000264 -3.076099 0.646540
8 -0.000278 -2.432481 -0.472098
7 -0.000039 1.279867 -0.040120
8 0.000872 -2.599721 1.775068
1 0.000145 -4.178479 0.493719

CNC-II-H$^-$

1 1
28 -0.000013 -0.987497 -0.000146
7 2.218714 0.631400 0.000045
7 -2.218704 0.631407 -0.000442
7 -3.075951 -1.331934 0.000181
7 3.075948 -1.331944 0.000026
6 1.890747 -0.712165 0.000222
6 1.163908 1.554822 -0.000111
6 -1.163898 1.554830 -0.000401
6 -1.890745 -0.712155 -0.000145
6 -4.127609 -0.420713 0.000084
1 -5.157891 -0.747614 0.000317
6 -3.590173 0.820556 -0.000274

1 -4.046911 1.799975 -0.000480
6 -3.267845 -2.773502 0.000432
1 -2.287327 -3.252533 0.000890
1 -3.824488 -3.071363 -0.892116
1 -3.825091 -3.070955 0.892732
6 -1.222770 2.938619 0.000206
1 -2.169729 3.468082 0.000463
6 0.000013 3.612547 0.000583
1 0.000014 4.699153 0.001063
6 1.222788 2.938615 0.000523
1 2.169751 3.468067 0.001019
6 3.590184 0.820541 -0.000252
1 4.046936 1.799955 -0.000401
6 4.127613 -0.420730 -0.000239
1 5.157895 -0.747625 -0.000386
6 3.267837 -2.773512 0.000323
1 3.824357 -3.071059 0.893058
1 3.825225 -3.071272 -0.891784
1 2.287320 -3.252544 -0.000065
7 0.000006 0.913768 -0.000760
1 -0.000074 -2.455760 0.000734

CNC-0

0 1
28 -0.000009 -1.030199 0.040310
7 -2.205324 0.617060 -0.116759
7 2.205330 0.617029 -0.116895
7 3.098177 -1.330106 0.026866
7 -3.098190 -1.330080 0.026805
6 -1.878962 -0.731369 0.064356
6 -1.155436 1.547009 -0.133422
6 1.155456 1.546997 -0.133510
6 1.878949 -0.731387 0.064276
6 4.131311 -0.416318 -0.134955
1 5.166725 -0.726395 -0.176946
6 3.574260 0.813595 -0.215352
1 4.018010 1.790048 -0.350905
6 3.302955 -2.757785 0.167108
1 2.354881 -3.208205 0.475399
1 4.067269 -2.956711 0.924646
1 3.617678 -3.200221 -0.783399
6 1.216426 2.888669 0.210764
1 2.164864 3.379096 0.412298
6 0.000038 3.568019 0.329890
1 0.000055 4.621057 0.598035
6 -1.216364 2.888681 0.210867
1 -2.164781 3.379116 0.412483
6 -3.574245 0.813635 -0.215340
1 -4.017978 1.790097 -0.350885
6 -4.131308 -0.416277 -0.135042
1 -5.166719 -0.726353 -0.177123
6 -3.303018 -2.757748 0.167083
1 -3.618393 -3.200079 -0.783256
1 -4.066856 -2.956668 0.925108
1 -2.354793 -3.208273 0.474744
7 -0.000004 0.931059 -0.421333

CNC-I + CO_2

1 2
28 -0.017547 -0.589246 -0.340471

7 2.342031 0.878988 -0.026925
7 0.149044 1.362475 -0.025452
7 -2.094766 1.264778 -0.063993
7 -3.189769 -0.549512 -0.347791
7 3.113983 -1.099270 -0.272779
6 1.949239 -0.434598 -0.230423
6 1.358505 1.881047 0.090452
6 -0.954468 2.082405 0.070799
6 -1.929422 -0.093250 -0.284629
6 -4.123475 0.464041 -0.167604
1 -5.186671 0.269141 -0.187529
6 -3.433989 1.613329 0.011144
1 -3.768332 2.627665 0.176639
6 -3.544182 -1.947612 -0.530315
1 -2.703160 -2.466104 -0.995494
1 -4.417598 -2.019538 -1.182836
1 -3.773823 -2.410678 0.434599
6 -0.900055 3.452216 0.285792
1 -1.795621 4.060217 0.363107
6 0.375933 4.008280 0.400977
1 0.467458 5.077485 0.572492
6 1.538318 3.239450 0.309877
1 2.524196 3.682545 0.408929
6 3.720258 0.996959 0.051445
1 4.219999 1.942335 0.208990
6 4.205864 -0.255121 -0.104650
1 5.220802 -0.627591 -0.111819
6 3.232634 -2.535020 -0.460396
1 3.748084 -2.981686 0.394236
1 3.795143 -2.748808 -1.373510
1 2.228853 -2.957142 -0.543827
6 -0.511818 -3.302436 0.903374
8 -0.358033 -3.608717 -0.213262
8 -0.668433 -3.012446 2.019855

CNC-III-H$^-$

2 2
28 0.000000 -0.998406 0.025789
7 -2.226225 0.632713 -0.009523
7 2.226225 0.632713 -0.009516
7 3.095867 -1.334226 -0.003909
7 -3.095867 -1.334226 -0.003909
6 -1.924868 -0.709220 0.005565
6 -1.169260 1.561063 -0.011490
6 1.169260 1.561063 -0.011485
6 1.924868 -0.709219 0.005577
6 4.140057 -0.417451 -0.023122
1 5.171255 -0.740731 -0.033799
6 3.596366 0.822924 -0.025957
1 4.048005 1.804625 -0.039672
6 3.282698 -2.779336 -0.000787
1 2.300842 -3.255356 0.018360
1 3.855344 -3.068460 0.883499
1 3.823596 -3.075565 -0.902697
6 1.225813 2.942530 0.015130
1 2.171061 3.474372 0.032767
6 0.000000 3.613017 0.025754
1 -0.000001 4.699142 0.049716
6 -1.225814 2.942530 0.015126
1 -2.171062 3.474371 0.032762

6 -3.596366 0.822924 -0.025941
1 -4.048006 1.804625 -0.039643
6 -4.140057 -0.417451 -0.023100
1 -5.171255 -0.740731 -0.033764
6 -3.282697 -2.779337 -0.000813
1 -3.823539 -3.075559 -0.902760
1 -3.855400 -3.068467 0.883433
1 -2.300842 -3.255357 0.018392
7 0.000000 0.931587 -0.032694
1 0.000001 -2.445683 0.061424

CNC-I

1 2
28 -0.000029 -1.088841 -0.001049
7 2.227217 0.606221 -0.000476
7 -2.227210 0.606232 -0.000932
7 -3.168883 -1.312649 0.000717
7 3.168894 -1.312654 0.000419
6 1.949326 -0.752136 -0.000293
6 1.160927 1.527518 -0.000740
6 -1.160918 1.527521 -0.001031
6 -1.949317 -0.752128 -0.000142
6 -4.183778 -0.362266 0.000510
1 -5.227618 -0.643938 0.001107
6 -3.590810 0.852676 -0.000476
1 -4.005564 1.850765 -0.000949
6 -3.413409 -2.744703 0.001818
1 -2.451194 -3.260347 0.002538
1 -3.979370 -3.028129 -0.890003
1 -3.979923 -3.026611 0.893758
6 -1.224135 2.913955 0.000773
1 -2.168624 3.448628 0.001725
6 0.000010 3.586820 0.001584
1 0.000009 4.673666 0.002991
6 1.224151 2.913952 0.001123
1 2.168645 3.448617 0.002372
6 3.590815 0.852670 0.000114
1 4.005573 1.850758 0.000174
6 4.183786 -0.362272 0.000673
1 5.227628 -0.643936 0.001300
6 3.413431 -2.744711 0.000989
1 3.978312 -3.027241 0.893779
1 3.981055 -3.027455 -0.889978
1 2.451223 -3.260366 -0.000432
7 0.000006 0.897387 -0.002361

CO_2

0 1
6 0.000000 0.000000 0.000063
8 0.000000 0.000000 -1.164657
8 0.000000 0.000000 1.164610

CO

0 1
6 0.000000 0.000000 -0.649857
8 0.000000 0.000000 0.487393

H_2O

0 1
8 0.000000 0.000000 0.119235

1 0.000000 0.755821 -0.476941

1 0.000000 -0.755821 -0.476941

TS-CCC-III-H-CO_2

1 2

28 0.000981 -0.596487 -0.275186

7 2.279289 1.063943 -0.071686

7 -2.291638 1.043504 -0.070029

7 -3.087555 -0.925208 -0.398568

7 3.091497 -0.898121 -0.400819

6 1.933732 -0.239045 -0.284652

6 1.192941 1.961277 0.078805

6 -1.213137 1.950294 0.079358

6 -1.935146 -0.256607 -0.282480

6 -4.163270 -0.060978 -0.258852

1 -5.182615 -0.414676 -0.323919

6 -3.661177 1.184285 -0.053392

1 -4.152028 2.135687 0.093681

6 -3.214441 -2.363002 -0.591434

1 -2.312872 -2.735127 -1.082113

1 -4.083898 -2.562608 -1.220908

1 -3.339852 -2.860656 0.374789

6 -1.244988 3.326000 0.275782

1 -2.183119 3.870466 0.348763

6 -0.019315 3.993122 0.375582

1 -0.024212 5.068680 0.532292

6 1.212394 3.337219 0.275508

1 2.145526 3.890250 0.348169

6 3.647650 1.215861 -0.054868

1 4.130658 2.171149 0.093088

6 4.160084 -0.025098 -0.260736

1 5.182361 -0.370288 -0.325427

6 3.230586 -2.334526 -0.594826

1 3.402177 -2.826721 0.367093

1 4.075729 -2.525523 -1.259235

1 2.314088 -2.719831 -1.046355

6 0.022398 -2.719749 0.981449

8 0.008697 -1.710073 1.640461

8 0.041800 -3.890275 0.844283

6 -0.007109 1.288218 -0.002551

1 0.008233 -2.148819 -0.581118

TS-CNC-II-H-CO_2

1 1

28 0.000009 -0.527015 -0.073935

7 2.226327 1.081565 -0.035905

7 -0.000071 1.331333 -0.023774

7 -2.226454 1.081352 -0.035886

7 -3.069624 -0.887164 -0.115442

7 3.069681 -0.886871 -0.115445

6 1.897923 -0.249291 -0.096220

6 1.165815 1.985895 0.002191

6 -1.166022 1.985781 0.002202

6 -1.897926 -0.249475 -0.096189

6 -4.126183 0.017900 -0.063416

1 -5.153854 -0.316625 -0.072127

6 -3.599876 1.262984 -0.014566

1 -4.061662 2.238853 0.025725

6 -3.242101 -2.334105 -0.134891

1 -4.200852 -2.565862 -0.602241

1 -3.227511 -2.727032 0.885198

1 -2.438923 -2.789241 -0.717597

6 -1.218546 3.366344 0.061575

1 -2.169498 3.888122 0.083284

6 -0.000201 4.043729 0.091430

1 -0.000255 5.128914 0.138300

6 1.218211 3.366464 0.061562

1 2.169116 3.888329 0.083260

6 3.599729 1.263325 -0.014538

1 4.061424 2.239237 0.025778

6 4.126153 0.018290 -0.063379

1 5.153855 -0.316139 -0.072062

6 3.242289 -2.333796 -0.134902

1 3.227674 -2.726733 0.885184

1 4.201087 -2.565461 -0.602204

1 2.439179 -2.788999 -0.717651

6 0.000203 -2.890204 0.108729

8 0.000070 -2.370127 1.243646

8 0.000438 -4.040566 -0.297451

1 0.000082 -2.109941 -0.814606

CN-CCC-III-CO

2 2

28 1.116016 -0.042851 -0.007660

7 -0.631047 -2.266889 0.018090

7 -0.472270 2.281313 0.018129

7 1.537385 3.024479 0.041104

7 1.379270 -3.092032 0.041677

6 0.746896 -1.913257 0.018082

6 -1.483322 -1.173627 0.009345

6 -1.402734 1.228618 0.009823

6 0.835148 1.883887 0.017858

6 0.687591 4.120173 0.054559

1 1.072855 5.129770 0.074680

6 -0.586395 3.652875 0.040214

1 -1.537950 4.164301 0.046218

6 2.990872 3.133580 0.046405

1 3.402258 2.601496 0.907457

1 3.255848 4.188409 0.125553

1 3.399492 2.735938 -0.886078

6 -2.779325 1.290834 -0.012207

1 -3.318238 2.234650 -0.025941

6 -3.501900 0.063120 -0.019718

6 -2.881959 -1.180384 -0.007602

1 -3.457188 -2.101573 -0.014258

6 -0.798748 -3.596823 0.034391

1 -1.762555 -4.087284 0.037544

6 0.480145 -4.131761 0.050959

1 0.799226 -5.166179 0.069365

6 2.832773 -3.271754 0.051373

1 3.251439 -2.877975 -0.877027

1 3.044243 -4.338863 0.117889

1 3.253099 -2.765268 0.922468

6 2.959068 -0.056547 -0.108777

8 4.092103 -0.066278 -0.195882

6 -0.742276 0.009807 0.016959

6 -4.930140 0.126527 -0.046268

7 -6.090762 0.181847 -0.068814

CN-CCC-III-COOH$^-$

1 2

28 0.991648 -0.000769 -0.336234

7 -0.631382 2.279499 -0.139036

7 -0.633553 -2.279300 -0.137187

7 1.352713 -3.079233 -0.272841

7 1.355870 3.077207 -0.273479

6 0.683619 1.920009 -0.263642

6 -1.550111 1.206793 -0.083280

6 -1.551229 -1.205667 -0.082153

6 0.681800 -1.921271 -0.262514

6 0.482025 -4.152711 -0.153224

1 0.840344 -5.172469 -0.148690

6 -0.774874 -3.648148 -0.066622

1 -1.735052 -4.134938 0.026957

6 2.801100 -3.209770 -0.343449

1 3.215374 -2.330233 -0.838334

1 3.050609 -4.104196 -0.917820

1 3.217190 -3.295632 0.664903

6 -2.930110 -1.238986 0.056294

1 -3.491447 -2.167252 0.121427

6 -3.592739 0.001611 0.115920

6 -2.928949 1.241534 0.055209

1 -3.489431 2.170367 0.119584

6 -0.771212 3.648502 -0.068483

1 -1.730900 4.136351 0.024579

6 0.486311 4.151660 -0.154327

1 0.845769 5.171017 -0.149478

6 2.804508 3.206010 -0.342138

1 3.219390 3.290237 0.666863

1 3.055892 4.100796 -0.915128

1 3.218360 2.326570 -0.837581

6 2.486664 0.000490 0.863804

8 3.632110 -0.003760 0.169373

8 2.394904 0.004937 2.060647

6 -0.889296 0.000217 -0.172844

1 4.382805 -0.002470 0.800600

6 -5.016057 0.002343 0.256233

7 -6.173626 0.003005 0.369372

CN-CCC-III-CO_2^{2-}

0 2

28 -0.993830 0.000013 -0.109264

7 0.650502 -2.277058 -0.061008

7 0.650563 2.277044 -0.061144

7 -1.322833 3.109769 -0.084509

7 -1.322911 -3.109736 -0.084524

6 -0.680380 -1.926179 -0.084002

6 1.571649 -1.198788 -0.057799

6 1.571681 1.198750 -0.057877

6 -0.680328 1.926197 -0.084116

6 -0.430306 4.171415 -0.053109

1 -0.768624 5.198227 -0.049901

6 0.819572 3.644564 -0.039297

1 1.791620 4.116804 -0.025388

6 -2.768345 3.272304 -0.063456

1 -3.229795 2.443264 -0.603254

1 -3.028444 4.212845 -0.554241

1 -3.134584 3.289840 0.967567

6 2.955157 1.239689 0.021963

1 3.519681 2.168024 0.066507

6 3.626012 -0.000044 0.051231
6 2.955124 -1.239760 0.022050
1 3.519621 -2.168108 0.066663
6 0.819480 -3.644583 -0.039257
1 1.791517 -4.116845 -0.025329
6 -0.430408 -4.171405 -0.053189
1 -0.768751 -5.198210 -0.050072
6 -2.768426 -3.272251 -0.063526
1 -3.134687 -3.289952 0.967486
1 -3.028530 -4.212710 -0.554468
1 -3.229850 -2.443117 -0.603200
6 -2.974862 0.000042 0.302006
8 -3.452838 -0.000005 -0.827109
8 -3.262637 0.000072 1.479422
6 0.890748 -0.000012 -0.118468
6 5.051455 -0.000063 0.132286
7 6.213954 -0.000050 0.197737

CN-CCC-III-HCOO$^-$

1 2
28 -1.042734 0.000070 -0.216739
7 0.621574 2.288750 -0.109782
7 0.621360 -2.288776 -0.109967
7 -1.366540 -3.090518 -0.215919
7 -1.366245 3.090676 -0.215894
6 -0.691440 1.938211 -0.212025
6 1.520617 1.205680 -0.057664
6 1.520500 -1.205791 -0.057760
6 -0.691621 -1.938119 -0.212266
6 -0.490095 -4.162504 -0.114901
1 -0.847829 -5.182495 -0.107807
6 0.767983 -3.657996 -0.048183
1 1.730234 -4.143285 0.028906
6 -2.817098 -3.226384 -0.257626
1 -3.207082 -3.333441 0.759077
1 -3.073082 -4.112518 -0.841675
1 -3.244186 -2.337533 -0.723330
6 2.903347 -1.236141 0.032688
1 3.460456 -2.168289 0.069649
6 3.570593 -0.000160 0.075616
6 2.903467 1.235891 0.032780
1 3.460665 2.167983 0.069807
6 0.768339 3.657967 -0.048264
1 1.730639 4.143173 0.028731
6 -0.489693 4.162588 -0.115015
1 -0.847328 5.182615 -0.108027
6 -2.816796 3.226647 -0.257532
1 -3.243941 2.338141 -0.723843
1 -3.072703 4.113198 -0.840979
1 -3.206798 3.333047 0.759234
6 -3.129568 0.000044 0.939656
8 -2.086084 -0.000146 1.638952
8 -3.044999 0.000204 -0.325986
6 0.848121 -0.000022 -0.101642
1 -4.121862 0.000043 1.418745
6 4.998099 -0.000233 0.170441
7 6.158352 -0.000294 0.246799

CN-CCC-III-H$^-$

1 2

28 0.000205 -1.421807 0.000198
7 2.281064 0.244039 -0.000348
7 -2.281058 0.243490 -0.000335
7 -3.092502 -1.747118 0.000294
7 3.092835 -1.746450 0.000281
6 1.933364 -1.081289 -0.000163
6 1.203259 1.166477 -0.000606
6 -1.203470 1.166163 -0.000599
6 -1.933130 -1.081786 -0.000151
6 -4.160950 -0.863507 0.000218
1 -5.183059 -1.215117 0.000482
6 -3.649126 0.394283 -0.000105
1 -4.132770 1.360665 -0.000194
6 -3.244468 -3.194363 0.000052
1 -2.251123 -3.646908 0.000504
1 -3.793170 -3.503995 -0.892988
1 -3.794118 -3.504232 0.892429
6 -1.240930 2.552162 -0.000168
1 -2.168744 3.118093 0.000172
6 -0.000362 3.218780 -0.000062
6 1.240380 2.552479 -0.000181
1 2.168057 3.118634 0.000155
6 3.649105 0.395051 -0.000174
1 4.132590 1.361513 -0.000305
6 4.161133 -0.862657 0.000297
1 5.183303 -1.214091 0.000645
6 3.245047 -3.193670 0.000049
1 3.794626 -3.503443 0.892503
1 3.793926 -3.503200 -0.892917
1 2.251769 -3.646366 0.000364
6 -0.000022 0.498374 -0.001030
1 0.000612 -2.946381 0.001960
6 -0.000553 4.648939 0.000409
7 -0.000810 5.812155 0.000810

CN-CCC-I

0 2
28 -0.000017 -1.429020 -0.051379
7 -2.277118 0.201365 -0.111492
7 2.277130 0.201276 -0.111559
7 3.155665 -1.743461 0.079343
7 -3.155761 -1.743328 0.079335
6 -1.949176 -1.137579 0.011909
6 -1.194856 1.128327 -0.194210
6 1.194903 1.128285 -0.194259
6 1.949113 -1.137643 0.011916
6 4.199907 -0.832471 0.012071
1 5.234881 -1.144225 0.049142
6 3.642312 0.398334 -0.102051
1 4.094198 1.376967 -0.186154
6 3.345328 -3.174856 0.218070
1 2.362443 -3.644635 0.307652
1 3.935960 -3.392859 1.112797
1 3.861299 -3.577769 -0.658677
6 1.240849 2.502666 -0.017319
1 2.166826 3.061811 0.103511
6 0.000065 3.177532 0.028343
6 -1.240744 2.502712 -0.017265
1 -2.166697 3.061888 0.103609
6 -3.642290 0.398500 -0.101962

1 -4.094118 1.377168 -0.185978
6 -4.199954 -0.832280 0.012084
1 -5.234944 -1.143979 0.049155
6 -3.345494 -3.174729 0.217919
1 -3.860902 -3.577649 -0.659159
1 -3.936700 -3.392734 1.112264
1 -2.362662 -3.644501 0.308118
6 0.000007 0.455051 -0.371456
6 0.000093 4.593990 0.188250
7 0.000157 5.752439 0.317242

NMe_2-CCC-III-CO

2 2
28 1.457770 -0.000096 0.000848
7 -0.201376 2.276719 -0.026080
7 -0.201826 -2.276569 -0.030203
7 1.788009 -3.072820 -0.035927
7 1.788615 3.072593 -0.030764
6 1.119577 1.911127 -0.017592
6 -1.109614 1.205654 -0.024170
6 -1.109844 -1.205333 -0.024769
6 1.119204 -1.911239 -0.022130
6 0.909434 -4.146515 -0.051065
1 1.266588 -5.166549 -0.064412
6 -0.351075 -3.644948 -0.046992
1 -1.315279 -4.132208 -0.056965
6 3.238162 -3.216940 -0.028679
1 3.669533 -2.707911 -0.893962
1 3.479652 -4.278840 -0.087963
1 3.650362 -2.812350 0.899170
6 -2.477773 -1.248382 -0.011209
1 -3.009493 -2.193578 -0.011675
6 -3.187246 0.000435 0.001630
6 -2.477545 1.249097 -0.011358
1 -3.008444 2.194665 -0.002217
6 -0.350359 3.645133 -0.042603
1 -1.314471 4.132562 -0.052985
6 0.910246 4.146460 -0.045839
1 1.267611 5.166426 -0.058611
6 3.238787 3.216530 -0.023575
1 3.651208 2.810161 0.903380
1 3.480354 4.278521 -0.080840
1 3.669954 2.709157 -0.889944
6 3.281688 -0.000278 0.104621
8 4.417169 -0.000297 0.194946
6 -0.402563 0.000096 -0.028727
7 -4.530623 0.000231 0.033726
6 -5.280589 -1.251607 0.084555
1 -5.090507 -1.845838 -0.815588
1 -4.994006 -1.831994 0.967563
1 -6.344089 -1.026870 0.140944
6 -5.282966 1.251531 0.030631
1 -5.059797 1.832179 0.932418
1 -5.031282 1.845793 -0.853297
1 -6.347545 1.025742 0.010044

NMe_2-CCC-III-$COOH^-$

1 2
28 1.281632 0.000078 -0.010671
7 -0.365153 2.274226 -0.037278

7 -0.365072 -2.274142 -0.039387
7 1.619000 -3.084605 -0.052982
7 1.618908 3.084750 -0.048187
6 0.967266 1.910169 -0.038759
6 -1.283295 1.205531 -0.036179
6 -1.283245 -1.205480 -0.035757
6 0.967347 -1.910057 -0.041430
6 0.733629 -4.154871 -0.051409
1 1.082644 -5.177956 -0.061435
6 -0.521689 -3.643452 -0.044172
1 -1.488697 -4.125757 -0.049566
6 3.066107 -3.242874 -0.028003
1 3.526243 -2.442420 -0.609758
1 3.321324 -4.207188 -0.472080
1 3.433191 -3.209631 1.001684
6 -2.650985 -1.251293 -0.013612
1 -3.189219 -2.193052 -0.005305
6 -3.360263 0.000030 0.000031
6 -2.651040 1.251345 -0.014847
1 -3.188937 2.193174 0.000341
6 -0.521803 3.643537 -0.040460
1 -1.488817 4.125823 -0.046133
6 0.733509 4.154992 -0.045954
1 1.082496 5.178099 -0.054370
6 3.065998 3.243000 -0.022119
1 3.432646 3.206956 1.007624
1 3.321355 4.208533 -0.463447
1 3.526442 2.444181 -0.605879
6 3.171407 -0.000053 0.202774
8 3.936695 0.000663 -0.939397
8 3.747992 -0.000854 1.278742
6 -0.572569 0.000039 -0.046889
7 -4.705149 -0.000131 0.034617
1 4.867845 0.000616 -0.639160
6 -5.453627 -1.251657 0.084025
1 -5.263880 -1.851833 -0.812569
1 -5.176403 -1.833652 0.969555
1 -6.518152 -1.027574 0.134911
6 -5.455713 1.251016 0.036545
1 -5.233697 1.834904 0.936909
1 -5.212345 1.849687 -0.847322
1 -6.521184 1.026196 0.019841

NMe_2-CCC-III-CO_2^{2-}

0 2
28 1.344844 0.001278 -0.165373
7 -0.319000 2.270847 -0.128781
7 -0.313426 -2.272372 -0.127511
7 1.659323 -3.108981 -0.092178
7 1.651414 3.112408 -0.084486
6 1.012848 1.926120 -0.125409
6 -1.234032 1.181707 -0.163512
6 -1.231234 -1.185461 -0.160424
6 1.017541 -1.924258 -0.126954
6 0.764727 -4.169239 -0.061731
1 1.101176 -5.196393 -0.034539
6 -0.484074 -3.638340 -0.084310
1 -1.457117 -4.109018 -0.084086
6 3.103263 -3.271399 -0.037975
1 3.575827 -2.413324 -0.520014

1 3.382067 -4.185389 -0.567942

1 3.441447 -3.340811 1.000804

6 -2.613826 -1.233493 -0.053697

1 -3.135637 -2.182892 0.021593

6 -3.326560 -0.004136 -0.032669

6 -2.616936 1.226780 -0.058815

1 -3.140342 2.175182 0.017105

6 -0.493364 3.636171 -0.081016

1 -1.467638 4.104304 -0.081529

6 0.753979 4.170216 -0.052817

1 1.087659 5.198134 -0.020718

6 3.094758 3.278373 -0.024969

1 3.429621 3.342754 1.015201

1 3.372666 4.196102 -0.548892

1 3.571036 2.424300 -0.510449

6 3.254152 0.003174 0.447231

8 3.799082 0.004963 -0.659111

8 3.516070 0.002457 1.632755

6 -0.535629 -0.001100 -0.256805

7 -4.705906 -0.006671 0.027974

6 -5.412004 1.239245 0.236699

1 -5.160195 1.718371 1.196754

1 -5.196727 1.956592 -0.565573

1 -6.487192 1.047295 0.222952

6 -5.402311 -1.244952 0.305685

1 -5.225383 -1.989942 -0.481104

1 -5.105963 -1.691710 1.268260

1 -6.476792 -1.051752 0.337282

NMe_2-CCC-III-$HCOO^-$

1 2

28 1.293046 -0.000560 -0.217827

7 -0.338828 -2.282446 -0.106383

7 -0.337915 2.282084 -0.107578

7 1.648149 3.076640 -0.228095

7 1.647265 -3.077742 -0.221699

6 0.982545 -1.914999 -0.196881

6 -1.242185 -1.207526 -0.059832

6 -1.241545 1.207503 -0.058224

6 0.983128 1.914130 -0.200687

6 0.773620 4.154432 -0.147442

1 1.131670 5.174490 -0.156806

6 -0.483979 3.653680 -0.072744

1 -1.444851 4.143320 -0.005417

6 3.096829 3.210996 -0.290286

1 3.502292 3.362448 0.714900

1 3.349553 4.069993 -0.915949

1 3.512106 2.298284 -0.719672

6 -2.605858 1.248559 0.032999

1 -3.138438 2.192857 0.067415

6 -3.316126 0.000395 0.073008

6 -2.606621 -1.248023 0.029686

1 -3.139041 -2.192135 0.069316

6 -0.485395 -3.653964 -0.070568

1 -1.446580 -4.143225 -0.005025

6 0.772217 -4.155178 -0.141817

1 1.129995 -5.175344 -0.149232

6 3.096073 -3.212618 -0.279725

1 3.512733 -2.301721 -0.711617

1 3.350146 -4.074064 -0.901455

1 3.498928 -3.360280 0.727066
6 3.799385 0.000757 0.753591
8 3.269972 0.002172 1.863395
8 3.214154 -0.000766 -0.387757
6 -0.526948 -0.000157 -0.112727
1 4.912420 0.000603 0.673734
7 -4.657960 0.000808 0.154089
6 -5.408601 -1.250388 0.171510
1 -5.184164 -1.847658 -0.718219
1 -5.166653 -1.835276 1.066083
1 -6.474052 -1.025209 0.177973
6 -5.403869 1.253169 0.223770
1 -5.094481 1.839564 1.095529
1 -5.244922 1.847580 -0.682661
1 -6.465969 1.030186 0.313950

NMe_2-CCC-III-H^-

1 2
28 -1.730939 0.000003 -0.001578
7 -0.098943 -2.274119 -0.002601
7 -0.098938 2.274112 0.002111
7 -2.089607 3.071374 0.002997
7 -2.089619 -3.071364 -0.001280
6 -1.430287 -1.901891 -0.002253
6 0.820808 -1.207062 -0.001404
6 0.820809 1.207054 0.000088
6 -1.430286 1.901896 0.001375
6 -1.210638 4.147859 0.004624
1 -1.567311 5.168444 0.006055
6 0.047956 3.644727 0.003997
1 1.011328 4.134400 0.004778
6 -3.534727 3.227783 0.002042
1 -3.989011 2.235294 0.002236
1 -3.846428 3.777016 -0.890606
1 -3.847448 3.777829 0.893821
6 2.188631 1.251500 0.000662
1 2.727210 2.192995 0.006817
6 2.897808 -0.000006 -0.000262
6 2.188632 -1.251511 -0.001257
1 2.727209 -2.193011 -0.006821
6 0.047938 -3.644736 -0.001698
1 1.011306 -4.134418 -0.001472
6 -1.210660 -4.147857 -0.000906
1 -1.567340 -5.168440 0.000041
6 -3.534740 -3.227759 -0.000756
1 -3.846634 -3.777150 0.891725
1 -3.847279 -3.777642 -0.892703
1 -3.989017 -2.235267 -0.000818
6 0.110444 -0.000004 -0.001174
1 -3.272019 0.000019 -0.001732
7 4.243225 -0.000004 -0.000001
6 4.992652 1.251393 -0.026009
1 4.732849 1.840425 -0.912082
1 4.787830 1.845689 0.871495
1 6.057911 1.027068 -0.059553
6 4.992630 -1.251404 0.026611
1 4.733119 -1.839823 0.913192
1 4.787464 -1.846308 -0.870398
1 6.057907 -1.027084 0.059564

NMe_2-CCC-I

0 2

28 -1.778855 0.008808 -0.054722

7 -0.132212 2.266368 -0.176092

7 -0.156106 -2.265939 -0.174476

7 -2.088362 -3.145574 0.124752

7 -2.053939 3.166152 0.130609

6 -1.465608 1.952237 0.014363

6 0.778043 1.170321 -0.326334

6 0.765673 -1.179431 -0.323572

6 -1.486528 -1.937857 0.013281

6 -1.180287 -4.189661 0.024824

1 -1.487812 -5.224635 0.089510

6 0.042140 -3.630104 -0.157638

1 1.016144 -4.081912 -0.286133

6 -3.510858 -3.334444 0.331999

1 -3.972455 -2.351424 0.459756

1 -3.686385 -3.937933 1.227670

1 -3.960993 -3.835683 -0.530505

6 2.140235 -1.237853 -0.121551

1 2.644422 -2.185228 0.050813

6 2.862080 -0.015295 -0.094567

6 2.153427 1.214767 -0.126066

1 2.667180 2.156970 0.046280

6 0.080971 3.628200 -0.156016

1 1.059560 4.069704 -0.285342

6 -1.134788 4.200531 0.031383

1 -1.430955 5.238555 0.100267

6 -3.473488 3.370300 0.343453

1 -3.921138 3.878754 -0.516095

1 -3.638846 3.973440 1.241299

1 -3.945662 2.392240 0.470630

6 0.080356 -0.001113 -0.539221

7 4.246261 -0.023310 0.010660

6 4.935902 1.212582 0.310035

1 4.727315 1.974908 -0.450628

1 4.665773 1.632854 1.293678

1 6.013643 1.030926 0.301301

6 4.915743 -1.255815 0.366667

1 4.610936 -1.643000 1.353522

1 4.725078 -2.040421 -0.376173

1 5.994586 -1.082794 0.387937

NO_2-CCC-III-CO

2 2

28 1.382608 0.027709 -0.012790

7 -0.247021 -2.269518 0.024930

7 -0.322815 2.280974 0.027068

7 1.706071 3.072424 0.052049

7 1.751600 -3.043863 0.047188

6 1.066564 -1.892253 0.019791

6 -1.160581 -1.201469 0.018804

6 -1.197390 1.194307 0.016704

6 1.047780 1.900455 0.022913

6 0.833219 4.122404 0.067497

1 1.166235 5.152817 0.089877

6 -0.465333 3.605830 0.049644

1 -1.418364 4.118030 0.056485

6 3.163570 3.220010 0.058154

1 3.573666 2.700317 0.926261

1 3.397115 4.282095 0.127341
1 3.568518 2.819939 -0.873683
6 -2.594247 1.225129 -0.002666
1 -3.165388 2.147930 -0.012213
6 -3.215662 -0.009775 -0.011936
6 -2.540881 -1.244816 -0.000917
1 -3.101273 -2.174675 -0.013056
6 -0.381635 -3.637966 0.052673
1 -1.340898 -4.134869 0.063098
6 0.885623 -4.125362 0.066701
1 1.254319 -5.141033 0.090430
6 3.203374 -3.174426 0.047539
1 3.611793 -2.809122 -0.898245
1 3.453916 -4.230110 0.156232
1 3.626629 -2.623196 0.890669
6 3.227518 0.005262 -0.134136
8 4.359314 -0.008182 -0.233442
6 -0.480939 0.004771 0.024241
7 -4.684534 -0.037655 -0.043352
8 -5.227857 -1.129915 -0.029923
8 -5.269992 1.031457 -0.082924

NO_2-CCC-III-$COOH^-$

1 2
28 1.258763 -0.000157 -0.340137
7 -0.367411 2.278985 -0.160339
7 -0.367763 -2.279069 -0.160173
7 1.620143 -3.077022 -0.283516
7 1.620561 3.076778 -0.283548
6 0.948892 1.919526 -0.273254
6 -1.285864 1.206339 -0.111943
6 -1.286073 -1.206287 -0.111851
6 0.948560 -1.919720 -0.273035
6 0.749182 -4.151544 -0.175966
1 1.108029 -5.171125 -0.173081
6 -0.508850 -3.648295 -0.097296
1 -1.469683 -4.135689 -0.014088
6 3.069326 -3.204777 -0.343474
1 3.485605 -2.322222 -0.831308
1 3.324796 -4.096098 -0.920031
1 3.477727 -3.294509 0.667650
6 -2.665602 -1.240657 0.017646
1 -3.236023 -2.161759 0.080475
6 -3.307216 0.000200 0.069877
6 -2.665394 1.240944 0.017559
1 -3.235665 2.162142 0.080330
6 -0.508378 3.648214 -0.097240
1 -1.469167 4.135679 -0.013949
6 0.749692 4.151365 -0.175857
1 1.108645 5.170909 -0.172846
6 3.069741 3.204505 -0.343643
1 3.478182 3.294842 0.667411
1 3.325192 4.095479 -0.920746
1 3.486000 2.321652 -0.830949
6 2.710733 -0.000020 0.911009
8 3.877619 0.000017 0.255378
8 2.574592 0.000097 2.103251
6 -0.623595 -0.000031 -0.198091
7 -4.767397 0.000306 0.201357
8 -5.336935 1.080168 0.252601

8 -5.337051 -1.079486 0.252648

1 4.607346 0.000306 0.910857

NO_2-CCC-III-CO_2^{2-}

0 2

28 1.256635 -0.000013 -0.115176

7 -0.387892 2.277313 -0.073445

7 -0.387936 -2.277314 -0.073655

7 1.585129 -3.110648 -0.080285

7 1.585189 3.110611 -0.080380

6 0.943377 1.927008 -0.087893

6 -1.307858 1.199105 -0.077415

6 -1.307882 -1.199088 -0.077554

6 0.943341 -1.927036 -0.088011

6 0.691825 -4.171827 -0.052460

1 1.029669 -5.198759 -0.044129

6 -0.557937 -3.644667 -0.048998

1 -1.530496 -4.116001 -0.040578

6 3.030542 -3.273240 -0.047474

1 3.495986 -2.450238 -0.593048

1 3.293570 -4.219023 -0.526342

1 3.389450 -3.279648 0.986220

6 -2.690391 -1.240468 -0.000813

1 -3.264184 -2.160875 0.043850

6 -3.341257 0.000023 0.025059

6 -2.690366 1.240504 -0.000647

1 -3.264139 2.160918 0.044146

6 -0.557864 3.644673 -0.048934

1 -1.530414 4.116025 -0.040459

6 0.691907 4.171809 -0.052595

1 1.029770 5.198736 -0.044397

6 3.030605 3.273192 -0.047697

1 3.389576 3.279860 0.985974

1 3.293617 4.218852 -0.526817

1 3.496007 2.450049 -0.593092

6 3.235579 -0.000037 0.311388

8 3.711019 0.000002 -0.818258

8 3.519731 -0.000002 1.488950

6 -0.624844 0.000006 -0.138974

7 -4.796047 0.000037 0.105923

8 -5.373840 1.079744 0.138932

8 -5.373901 -1.079653 0.138453

NO_2-CCC-III-$HCOO^-$

1 2

28 -1.302953 0.000043 -0.219501

7 0.362359 2.288757 -0.122234

7 0.362268 -2.288741 -0.122346

7 -1.626157 -3.090614 -0.213239

7 -1.626029 3.090712 -0.213221

6 -0.951481 1.938341 -0.215523

6 1.260997 1.205950 -0.075955

6 1.260947 -1.205971 -0.076015

6 -0.951558 -1.938274 -0.215667

6 -0.748737 -4.162380 -0.117706

1 -1.106271 -5.182412 -0.107173

6 0.509772 -3.657849 -0.060395

1 1.472885 -4.142441 0.010183

6 -3.077051 -3.226763 -0.243737

1 -3.459217 -3.330904 0.776221

1 -3.337124 -4.114676 -0.823230
1 -3.507822 -2.339426 -0.708929
6 2.644175 -1.236856 0.006215
1 3.211505 -2.161297 0.040915
6 3.288541 -0.000055 0.043260
6 2.644226 1.236775 0.006279
1 3.211593 2.161192 0.041026
6 0.509926 3.657865 -0.060436
1 1.473061 4.142420 0.010087
6 -0.748563 4.162445 -0.117763
1 -1.106052 5.182493 -0.107288
6 -3.076920 3.226911 -0.243690
1 -3.507724 2.339713 -0.709117
1 -3.336956 4.114987 -0.822950
1 -3.459090 3.330800 0.776292
6 -3.379409 -0.000046 0.953188
8 -2.331025 -0.000188 1.645088
8 -3.302763 0.000094 -0.313139
6 0.587760 0.000004 -0.115772
1 -4.368368 -0.000069 1.438809
7 4.753409 -0.000088 0.131350
8 5.322221 -1.080191 0.165912
8 5.322261 1.079990 0.166054

NO_2-CCC-III-H^-

1 2
28 -1.693364 -0.000004 0.000488
7 -0.026932 -2.280984 0.000007
7 -0.027032 2.280993 -0.000036
7 -2.017240 3.093031 0.000041
7 -2.017061 -3.093191 -0.000340
6 -1.352624 -1.933544 0.000016
6 0.894885 -1.203512 0.000040
6 0.894838 1.203562 -0.000103
6 -1.352691 1.933451 0.000156
6 -1.133083 4.161100 -0.000161
1 -1.484258 5.183358 -0.000176
6 0.124529 3.648964 -0.000258
1 1.091372 4.131732 -0.000454
6 -3.464497 3.245581 0.000132
1 -3.917416 2.252413 -0.000218
1 -3.773858 3.795183 -0.892429
1 -3.773827 3.794621 0.893046
6 2.280552 1.241332 -0.000219
1 2.856348 2.161177 -0.000350
6 2.924802 0.000071 -0.000031
6 2.280605 -1.241215 0.000142
1 2.856446 -2.161032 0.000262
6 0.124745 -3.648945 -0.000313
1 1.091631 -4.131629 -0.000376
6 -1.132821 -4.161189 -0.000598
1 -1.483910 -5.183477 -0.000854
6 -3.464307 -3.245832 -0.000516
1 -3.773755 -3.795086 0.892226
1 -3.773497 -3.795255 -0.893247
1 -3.917302 -2.252700 -0.000709
6 0.226261 0.000009 0.000038
1 -3.216247 0.000316 0.000683
7 4.390456 0.000103 0.000035
8 4.963148 -1.079628 0.002326

8 4.963100 1.079859 -0.002193

NO_2-CCC-I

0 2

28 -1.690875 0.000095 -0.068222

7 -0.066513 2.276148 -0.133772

7 -0.066823 -2.276145 -0.133692

7 -2.009863 -3.148263 0.098701

7 -2.009405 3.148537 0.098780

6 -1.400991 1.945440 0.010438

6 0.854749 1.194307 -0.234690

6 0.854584 -1.194427 -0.234602

6 -1.401270 -1.945254 0.010373

6 -1.101761 -4.194940 0.024764

1 -1.415375 -5.228732 0.075585

6 0.128319 -3.641863 -0.114887

1 1.104668 -4.096118 -0.211251

6 -3.439585 -3.333371 0.260794

1 -3.904923 -2.349367 0.359218

1 -3.644269 -3.924273 1.158414

1 -3.858558 -3.847042 -0.609696

6 2.224654 -1.240089 -0.048742

1 2.789127 -2.159625 0.077056

6 2.885626 -0.000197 -0.006245

6 2.224836 1.239781 -0.048869

1 2.789467 2.159245 0.076755

6 0.128825 3.641837 -0.115000

1 1.105235 4.095947 -0.211432

6 -1.101165 4.195089 0.024758

1 -1.414652 5.228919 0.075582

6 -3.439084 3.333875 0.261000

1 -3.858051 3.847608 -0.609456

1 -3.643586 3.924817 1.158634

1 -3.904576 2.349948 0.359463

6 0.176180 -0.000015 -0.439847

7 4.321084 -0.000281 0.155464

8 4.903643 1.080801 0.219706

8 4.903498 -1.081426 0.219981

OMe-CCC-III-CO

2 2

28 -1.180385 0.272560 0.001190

7 -0.199883 -2.367304 -0.000011

7 1.028895 2.021444 0.000642

7 -0.682456 3.314839 -0.000196

7 -2.331608 -2.594770 -0.000016

6 -1.376324 -1.657991 0.000352

6 0.958394 -1.585997 0.000312

6 1.616767 0.760696 0.000764

6 -0.350431 2.021133 0.000619

6 0.452587 4.116749 -0.000656

1 0.377446 5.195071 -0.001132

6 1.536132 3.301822 -0.000182

1 2.595201 3.515782 -0.000276

6 -2.041709 3.844299 -0.000960

1 -2.568201 3.516168 -0.900402

1 -1.985694 4.933313 -0.000584

1 -2.569374 3.515682 0.897609

6 2.947444 0.439112 0.000313

1 3.726599 1.194618 0.000143

6 3.262615 -0.947386 -0.000205
6 2.264669 -1.977393 -0.000272
1 2.587743 -3.014363 -0.000879
6 -0.424595 -3.725360 -0.000812
1 0.373531 -4.453908 -0.001273
6 -1.773529 -3.866212 -0.000737
1 -2.393584 -4.751686 -0.001034
6 -3.768508 -2.344355 0.000106
1 -4.051108 -1.791157 0.899141
1 -4.284575 -3.305176 0.000089
1 -4.051273 -1.791042 -0.898804
6 -2.950526 0.763440 -0.000345
8 -4.046630 1.067578 -0.001773
6 0.601327 -0.223798 0.001139
6 5.607702 -0.496237 -0.000636
1 6.493759 -1.129909 -0.001028
1 5.590389 0.125354 -0.901327
1 5.590750 0.124785 0.900451
8 4.489436 -1.401304 -0.000695

OMe-CCC-III-COOH^{-}

1 2
28 1.067545 0.194051 -0.324389
7 -1.037350 2.043068 -0.145294
7 -0.006734 -2.395533 -0.148109
7 2.110991 -2.724672 -0.242229
7 0.713295 3.276507 -0.267583
6 0.325366 1.995132 -0.262176
6 -1.681408 0.783825 -0.104068
6 -1.141832 -1.553293 -0.108125
6 1.194756 -1.748383 -0.256453
6 1.504280 -3.967551 -0.125878
1 2.085405 -4.878751 -0.105835
6 0.164526 -3.760006 -0.064634
1 -0.662460 -4.450468 0.020333
6 3.552367 -2.524886 -0.277449
1 3.772650 -1.592563 -0.799777
1 4.015045 -3.359608 -0.807699
1 3.947451 -2.476234 0.741997
6 -2.471833 -1.894020 0.031228
1 -2.821814 -2.921020 0.096414
6 -3.412285 -0.841513 0.095837
6 -3.035643 0.514137 0.037932
1 -3.768684 1.312195 0.104702
6 -1.488995 3.342873 -0.073914
1 -2.535678 3.596598 0.014944
6 -0.381082 4.122715 -0.152065
1 -0.264714 5.197319 -0.145398
6 2.092960 3.735681 -0.336003
1 2.486023 3.893615 0.673061
1 2.128889 4.674736 -0.891759
1 2.693794 2.983838 -0.850170
6 2.567123 0.540977 0.816943
8 3.677076 0.804395 0.104208
8 2.522395 0.527194 2.019664
6 -0.753031 -0.229091 -0.215226
1 4.409780 0.982456 0.730615
8 -4.686952 -1.243293 0.224732
6 -5.701849 -0.257391 0.334395
1 -5.546727 0.377756 1.215469

1 -5.749388 0.369044 -0.565545

1 -6.642916 -0.799525 0.443152

OMe-CCC-III-CO_2^{2-}

0 2

28 1.087208 0.187272 -0.130879

7 -1.022839 2.046642 -0.079669

7 -0.037104 -2.392307 -0.082016

7 2.069709 -2.781355 -0.084263

7 0.717598 3.295168 -0.103359

6 0.351958 1.997858 -0.101101

6 -1.681718 0.787323 -0.084618

6 -1.168993 -1.534379 -0.089894

6 1.187204 -1.762878 -0.096172

6 1.426171 -4.010316 -0.052882

1 1.978691 -4.939572 -0.040185

6 0.091987 -3.763219 -0.052097

1 -0.756287 -4.433076 -0.041470

6 3.515742 -2.630323 -0.050053

1 3.788951 -1.699291 -0.550329

1 3.976089 -3.472109 -0.572548

1 3.872457 -2.610528 0.984486

6 -2.510125 -1.870091 0.005307

1 -2.872187 -2.894289 0.061152

6 -3.442406 -0.813477 0.044613

6 -3.049177 0.535233 0.013170

1 -3.775657 1.340831 0.070646

6 -1.489374 3.342379 -0.059470

1 -2.541956 3.587696 -0.046121

6 -0.387188 4.133865 -0.073744

1 -0.282906 5.210021 -0.071805

6 2.090380 3.774170 -0.090686

1 2.432290 3.927643 0.937698

1 2.143971 4.721431 -0.632237

1 2.728227 3.038057 -0.583763

6 2.988354 0.609644 0.368531

8 3.473128 0.715469 -0.758300

8 3.282362 0.677819 1.544091

6 -0.752129 -0.221088 -0.165189

8 -4.735374 -1.207277 0.130768

6 -5.730611 -0.208810 0.231504

1 -5.754735 0.432632 -0.660283

1 -6.685757 -0.731813 0.317067

1 -5.585937 0.418274 1.121677

OMe-CCC-III-$HCOO^-$

1 2

28 1.112623 0.235505 -0.198477

7 0.071751 -2.401533 -0.090552

7 -1.084864 2.024180 -0.107001

7 0.631036 3.308767 -0.195633

7 2.197069 -2.680320 -0.184281

6 1.254854 -1.732016 -0.184942

6 -1.071098 -1.576448 -0.050349

6 -1.674694 0.743244 -0.059095

6 0.274800 2.020610 -0.191792

6 -0.492064 4.120845 -0.111584

1 -0.407083 5.198446 -0.105195

6 -1.578899 3.309638 -0.056660

1 -2.634459 3.531820 0.007218

6 1.998512 3.810481 -0.221066
1 2.355251 3.968370 0.801392
1 2.018636 4.757279 -0.763882
1 2.634818 3.081291 -0.724503
6 -3.025785 0.431353 0.018240
1 -3.778449 1.213326 0.044907
6 -3.370431 -0.930535 0.060249
6 -2.397909 -1.950875 0.024328
1 -2.715157 -2.989821 0.056906
6 0.271969 -3.763377 -0.029847
1 -0.539382 -4.473539 0.041487
6 1.616627 -3.937850 -0.088366
1 2.219033 -4.835359 -0.078519
6 3.635213 -2.449010 -0.217187
1 3.832110 -1.505910 -0.728887
1 4.113330 -3.270112 -0.754675
1 4.027023 -2.403485 0.803568
6 3.202898 0.795972 0.823494
8 2.232840 0.547056 1.581837
8 3.058853 0.745575 -0.434273
6 -0.709429 -0.240506 -0.093634
1 4.185478 1.060526 1.248757
8 -4.637871 -1.368048 0.135906
6 -5.683378 -0.409649 0.189669
1 -5.586144 0.237488 1.070537
1 -5.708051 0.206968 -0.718060
1 -6.613043 -0.977014 0.262062

OMe-CCC-III-H$^-$

1 2
28 -1.047344 -1.107348 0.019529
7 1.766386 -1.350761 -0.011996
7 -1.663781 1.652022 -0.008732
7 -3.585234 0.689003 -0.004146
7 1.072276 -3.384734 -0.007392
6 0.633412 -2.120821 -0.004321
6 1.553674 0.053551 -0.001573
6 -0.244293 1.631234 -0.000455
6 -2.273447 0.425341 0.002520
6 -3.807305 2.057917 -0.021676
1 -4.808268 2.466044 -0.031705
6 -2.593318 2.666360 -0.023750
1 -2.320372 3.711939 -0.034386
6 -4.655006 -0.297417 -0.000751
1 -4.208855 -1.291644 0.062896
1 -5.237969 -0.209921 -0.921195
1 -5.305219 -0.126622 0.860810
6 0.640544 2.692948 0.003725
1 0.328572 3.734276 0.006075
6 2.019637 2.390079 0.005286
6 2.503545 1.068688 0.002721
1 3.567502 0.851729 0.004436
6 2.896941 -2.134220 -0.020786
1 3.896083 -1.722510 -0.028357
6 2.458551 -3.419612 -0.018927
1 2.998749 -4.355799 -0.026099
6 0.240224 -4.577931 -0.001684
1 0.468313 -5.178685 0.882440
1 0.436246 -5.165855 -0.902012
1 -0.806967 -4.270925 0.019794

6 0.206854 0.326925 0.002394

1 -2.056970 -2.259478 0.118419

8 2.825878 3.467999 0.009881

6 4.228263 3.262155 0.006129

1 4.551674 2.720246 -0.892164

1 4.683292 4.254272 0.008268

1 4.555614 2.714783 0.899684

OMe-CCC-I

0 2

28 -0.811976 1.298668 -0.033433

7 1.970127 1.008549 -0.141740

7 -1.973278 -1.248616 -0.126745

7 -3.703421 -0.002283 0.095514

7 1.778104 3.132650 0.077083

6 1.026531 2.008776 0.014133

6 1.481897 -0.333711 -0.242659

6 -0.570659 -1.510722 -0.232727

6 -2.354293 0.073157 0.027020

6 -4.156916 -1.310281 0.000868

1 -5.209954 -1.555169 0.034869

6 -3.060147 -2.097325 -0.133452

1 -2.965892 -3.169015 -0.242767

6 -4.577033 1.142600 0.265331

1 -3.954392 2.031082 0.401192

1 -5.212682 1.005384 1.145217

1 -5.210294 1.275631 -0.617202

6 0.074913 -2.722708 -0.028953

1 -0.440576 -3.669420 0.124919

6 1.483747 -2.702465 0.021507

6 2.216105 -1.504148 -0.037448

1 3.294075 -1.493462 0.104526

6 3.253165 1.512638 -0.156036

1 4.127878 0.886571 -0.266335

6 3.134178 2.857780 -0.024213

1 3.881130 3.639581 0.006699

6 1.238270 4.469354 0.235093

1 1.396864 5.057552 -0.674186

1 1.721880 4.974236 1.076537

1 0.165446 4.386087 0.429213

6 0.118822 -0.329777 -0.431616

8 2.060862 -3.921555 0.187870

6 3.464876 -3.977947 0.312778

1 3.817680 -3.432693 1.199613

1 3.725602 -5.033576 0.421154

1 3.970195 -3.576476 -0.576817

TS-CN-CCC-III-H-CO_2

1 2

28 -0.996770 -0.000150 -0.263163

7 0.660052 -2.285385 -0.130997

7 0.659441 2.285571 -0.131261

7 -1.317717 3.087200 -0.383161

7 -1.316765 -3.087710 -0.383170

6 -0.650250 -1.933755 -0.289637

6 1.565338 -1.205762 -0.019547

6 1.565026 1.206199 -0.019703

6 -0.650742 1.933506 -0.289699

6 -0.443871 4.160169 -0.283139

1 -0.795990 5.180645 -0.337836

6 0.806628 3.655251 -0.126138
1 1.765220 4.142555 -0.019996
6 -2.761579 3.219824 -0.522750
1 -3.159336 2.298123 -0.952325
1 -2.980657 4.058942 -1.185934
1 -3.216137 3.397107 0.456344
6 2.945675 1.238887 0.102328
1 3.506734 2.168585 0.143149
6 3.609529 0.000493 0.166665
6 2.945999 -1.238083 0.102500
1 3.507285 -2.167638 0.143473
6 0.807739 -3.655006 -0.125940
1 1.766474 -4.141973 -0.019537
6 -0.442551 -4.160366 -0.283077
1 -0.794308 -5.180963 -0.337836
6 -2.760509 -3.221033 -0.522974
1 -2.979096 -4.059206 -1.187514
1 -3.158848 -2.298889 -0.951052
1 -3.214930 -3.400109 0.455856
6 -3.069873 -0.000166 1.044645
8 -2.043473 -0.000324 1.681521
8 -4.245437 0.000040 0.948554
6 0.897654 0.000126 -0.062406
1 -2.555644 -0.000299 -0.507017
6 5.034112 0.000694 0.296727
7 6.192148 0.000855 0.403024

TS-NMe$_2$-CCC-III-H-CO$_2$

1 2

28 1.215197 -0.000200 -0.207937
7 -0.404504 2.276762 -0.098987
7 -0.405299 -2.276616 -0.099383
7 1.581845 -3.065088 -0.263985
7 1.583322 3.064605 -0.258386
6 0.917894 1.901451 -0.204409
6 -1.319622 1.209288 -0.030340
6 -1.319910 -1.208867 -0.028516
6 0.917069 -1.901727 -0.206723
6 0.710882 -4.145583 -0.189803
1 1.070160 -5.164729 -0.219962
6 -0.546450 -3.648357 -0.089055
1 -1.504988 -4.142153 -0.018139
6 3.028402 -3.197710 -0.344233
1 3.439248 -2.307862 -0.824479
1 3.274319 -4.079797 -0.939491
1 3.454704 -3.306046 0.657869
6 -2.685479 -1.250748 0.048658
1 -3.222992 -2.192661 0.066849
6 -3.393302 0.000565 0.088666
6 -2.685275 1.251597 0.045301
1 -3.222084 2.193740 0.068240
6 -0.545061 3.648552 -0.086727
1 -1.503517 4.142660 -0.016913
6 0.712697 4.145375 -0.184135
1 1.072489 5.164407 -0.211889
6 3.030145 3.196778 -0.334479
1 3.453538 3.304103 0.668968
1 3.278099 4.079301 -0.928251
1 3.442135 2.307215 -0.814271
6 3.907455 -0.000360 0.701659

8 3.373266 -0.001281 1.768645
8 4.885427 0.000650 0.020528
6 -0.612265 0.000109 -0.058168
1 2.768449 -0.000558 -0.419267
6 -5.486958 1.251924 0.171249
1 -5.244176 1.841997 1.062070
1 -5.263622 1.844026 -0.722290
1 -6.552346 1.026622 0.180064
6 -5.483929 -1.250965 0.222002
1 -5.325252 -1.840228 -0.687917
1 -5.176239 -1.843047 1.090382
1 -6.545763 -1.026923 0.312611
7 -4.736075 0.000712 0.160595

TS-NO_2-CCC-III-H-CO_2

1 2
28 1.260595 0.000006 -0.264959
7 -0.398073 2.285473 -0.146837
7 -0.398066 -2.285469 -0.146910
7 1.580627 -3.087950 -0.381406
7 1.580615 3.087969 -0.381315
6 0.913688 1.933962 -0.294468
6 -1.303548 1.206075 -0.044170
6 -1.303545 -1.206077 -0.044209
6 0.913694 -1.933949 -0.294528
6 0.705404 -4.160430 -0.287881
1 1.057499 -5.181100 -0.338902
6 -0.546188 -3.655018 -0.141879
1 -1.506124 -4.141325 -0.043483
6 3.025535 -3.221517 -0.509226
1 3.427399 -2.299633 -0.934517
1 3.249377 -4.060081 -1.171483
1 3.471644 -3.400184 0.473467
6 -2.685471 -1.239060 0.060462
1 -3.256496 -2.161266 0.094332
6 -3.327511 -0.000007 0.113887
6 -2.685475 1.239051 0.060502
1 -3.256502 2.161254 0.094403
6 -0.546201 3.655021 -0.141768
1 -1.506139 4.141321 -0.043356
6 0.705388 4.160443 -0.287759
1 1.057478 5.181116 -0.338752
6 3.025523 3.221547 -0.509135
1 3.471628 3.400230 0.473557
1 3.249359 4.060106 -1.171401
1 3.427394 2.299661 -0.934414
6 3.319549 -0.000015 1.059872
8 2.287367 -0.000015 1.688214
8 4.496211 -0.000026 0.976576
6 -0.634826 0.000001 -0.079118
1 2.821812 0.000010 -0.491159
7 -4.790416 -0.000011 0.224693
8 -5.359533 1.079908 0.268225
8 -5.359531 -1.079933 0.268172

TS-OMe-CCC-III-H-CO_2

1 2
28 1.076293 0.156413 -0.273016
7 -0.998577 2.074969 -0.128694
7 -0.114677 -2.407336 -0.126617

7 1.984275 -2.816541 -0.322948
7 0.785375 3.248354 -0.359065
6 0.354348 1.985100 -0.286700
6 -1.673275 0.833652 -0.032260
6 -1.211399 -1.518310 -0.036265
6 1.104795 -1.810650 -0.270653
6 1.332313 -4.036372 -0.210770
1 1.877169 -4.969604 -0.232384
6 0.004755 -3.778692 -0.088755
1 -0.844560 -4.438736 0.014405
6 3.429392 -2.671763 -0.427485
1 3.655394 -1.733190 -0.937782
1 3.830340 -3.507545 -1.003959
1 3.878178 -2.666610 0.570327
6 -2.556441 -1.814438 0.068189
1 -2.939213 -2.831183 0.101591
6 -3.462277 -0.734766 0.130617
6 -3.039634 0.605569 0.075268
1 -3.747836 1.427803 0.109429
6 -1.408431 3.389658 -0.101249
1 -2.443477 3.679646 0.009577
6 -0.279679 4.130861 -0.244423
1 -0.129971 5.200741 -0.279795
6 2.176635 3.659510 -0.484527
1 2.601749 3.849829 0.505642
1 2.226321 4.570595 -1.083961
1 2.736804 2.864269 -0.980631
6 3.186846 0.599665 0.949918
8 2.209722 0.398013 1.625443
8 4.328358 0.842213 0.786246
6 -0.773200 -0.207476 -0.075021
1 2.596131 0.455725 -0.608125
8 -4.752577 -1.095087 0.238202
6 -5.734341 -0.075219 0.327973
1 -5.566749 0.563782 1.204142
1 -5.753410 0.543678 -0.578488
1 -6.694310 -0.583974 0.433457

CN-CNC-II-CO

2 1
28 1.108732 -0.000012 -0.001822
7 -0.508721 -2.224976 0.018653
7 -0.508682 2.224980 0.018604
7 1.459997 3.074266 0.028584
7 1.459945 -3.074294 0.028556
6 0.824629 -1.904586 0.013992
6 -1.411982 -1.166632 0.014833
6 -1.411960 1.166652 0.014805
6 0.824664 1.904568 0.013995
6 0.550401 4.125819 0.041038
1 0.882125 5.154173 0.054415
6 -0.694804 3.596332 0.034296
1 -1.673839 4.053371 0.041399
6 2.909107 3.252605 0.029354
1 3.340929 2.766421 0.907248
1 3.124676 4.320437 0.071629
1 3.332148 2.839676 -0.889634
6 -2.792129 1.226973 -0.006466
6 -3.465876 0.000029 -0.016204
6 -2.792152 -1.226928 -0.006432
6 -0.694865 -3.596325 0.034360

1 -1.673908 -4.053348 0.041511
6 0.550332 -4.125833 0.041041
1 0.882039 -5.154192 0.054402
6 2.909051 -3.252661 0.029272
1 3.332073 -2.839687 -0.889705
1 3.124599 -4.320500 0.071473
1 3.340911 -2.766540 0.907183
6 2.895178 -0.000021 -0.089189
8 4.028658 0.000003 -0.158596
7 -0.763647 0.000004 0.028190
1 -3.321670 2.173730 -0.018582
1 -3.321711 -2.173675 -0.018522
6 -4.899164 0.000042 -0.045624
7 -6.059563 0.000054 -0.069938

CN-CNC-II-COOH$^-$

1 1
28 0.970427 0.000010 -0.021465
7 -0.662821 2.220278 -0.011882
7 -0.662793 -2.220270 -0.011711
7 1.292623 -3.091118 0.007184
7 1.292595 3.091129 0.007171
6 0.682484 1.901896 -0.000302
6 -1.578187 1.164793 -0.010760
6 -1.578169 -1.164796 -0.010662
6 0.682516 -1.901885 -0.000036
6 0.373621 -4.135674 -0.005058
1 0.692534 -5.168308 -0.000864
6 -0.863708 -3.591104 -0.014114
1 -1.847019 -4.039225 -0.017372
6 2.736730 -3.287546 -0.009885
1 3.115088 -3.207785 -1.032439
1 2.958613 -4.280953 0.383981
1 3.210470 -2.534928 0.623025
6 -2.961498 -1.230172 0.004753
6 -3.632763 -0.000016 0.010002
6 -2.961516 1.230151 0.004642
6 -0.863739 3.591113 -0.014008
1 -1.847050 4.039235 -0.017161
6 0.373590 4.135683 -0.004836
1 0.692497 5.168318 -0.000436
6 2.736708 3.287527 -0.009940
1 3.210441 2.535082 0.623186
1 2.958598 4.281044 0.383645
1 3.115075 3.207486 -1.032466
6 2.816815 0.000022 -0.086635
8 3.490494 0.000073 -1.096302
8 3.406686 -0.000054 1.139413
1 4.372722 -0.000029 0.985843
7 -0.941442 0.000002 -0.022466
1 -3.497237 2.173436 0.013326
1 -3.497209 -2.173462 0.013529
6 -5.066424 -0.000028 0.026490
7 -6.227546 -0.000040 0.039194

CN-CNC-II-CO_2^{2-}

0 1
28 -1.048943 -0.000031 0.060312
7 0.636415 -2.217935 0.059956
7 0.924537 0.000013 0.190892

7 0.636282 2.217950 0.059960
7 -1.299089 3.115224 -0.114065
7 -1.298907 -3.115307 -0.114064
6 -0.715293 -1.906802 -0.047150
6 1.554998 -1.162548 0.098443
6 1.554924 1.162615 0.098451
6 -0.715411 1.906748 -0.047164
6 -0.370856 4.149921 -0.053291
1 -0.672023 5.187530 -0.095096
6 0.853875 3.588203 0.049405
1 1.840080 4.025296 0.115499
6 -2.735117 3.321160 -0.221380
1 -3.182648 2.431537 -0.671762
1 -2.927733 4.192423 -0.852221
1 -3.170738 3.488926 0.768493
6 2.937332 1.231031 0.009410
6 3.610278 0.000097 -0.012447
6 2.937409 -1.230880 0.009401
6 0.854083 -3.588176 0.049383
1 1.840310 -4.025219 0.115476
6 -0.370617 -4.149957 -0.053345
1 -0.671726 -5.187581 -0.095182
6 -2.734929 -3.321298 -0.221351
1 -3.170550 -3.488938 0.768542
1 -2.927516 -4.192653 -0.852073
1 -3.182484 -2.431746 -0.671849
6 -2.933821 -0.000101 0.073238
8 -3.625193 0.000040 -0.951545
8 -3.193099 -0.000117 1.288872
1 3.474960 2.171888 -0.051226
1 3.475095 -2.171703 -0.051240
6 5.039688 0.000141 -0.100207
7 6.199684 0.000170 -0.168833

CN-CNC-II-HCOO$^-$

1 1
28 0.977148 -0.000017 -0.236101
7 -0.637787 -2.228628 -0.090836
7 -0.637758 2.228660 -0.090716
7 1.322996 3.079785 -0.210269
7 1.322955 -3.079771 -0.210458
6 0.695159 -1.904823 -0.199474
6 -1.536453 -1.166904 -0.038467
6 -1.536443 1.166928 -0.038423
6 0.695225 1.904810 -0.198607
6 0.417721 4.133217 -0.105393
1 0.748873 5.162098 -0.099679
6 -0.823507 3.601980 -0.031669
1 -1.799073 4.059318 0.049665
6 2.769121 3.252108 -0.274073
1 3.171727 3.378915 0.735184
1 2.995219 4.137900 -0.871116
1 3.205886 2.367012 -0.738171
6 -2.914828 1.226932 0.068075
6 -3.586840 0.000021 0.114399
6 -2.914843 -1.226901 0.068021
6 -0.823469 -3.601912 -0.030774
1 -1.798990 -4.059222 0.051298
6 0.417732 -4.133177 -0.104683
1 0.748970 -5.162025 -0.098431

6 2.769030 -3.252138 -0.275190
1 3.205570 -2.366655 -0.738752
1 2.994770 -4.137441 -0.873097
1 3.172190 -3.379789 0.733735
6 3.432658 0.000034 0.711918
8 2.829530 0.000002 -0.429912
7 -0.890831 0.000017 -0.099961
1 -3.444451 -2.172655 0.112783
1 -3.444470 2.172662 0.112916
6 -5.016386 0.000040 0.219141
7 -6.174459 -0.000064 0.301699
8 2.913603 -0.000142 1.821142
1 4.539509 0.000195 0.599644

CN-CNC-II-H$^-$

1 1
28 -0.000005 -1.398063 -0.000264
7 2.218955 0.219787 -0.000112
7 -2.218954 0.219796 -0.000374
7 -3.073563 -1.744330 0.000020
7 3.073559 -1.744341 -0.000053
6 1.889609 -1.125692 0.000024
6 1.166660 1.138702 -0.000217
6 -1.166656 1.138708 -0.000364
6 -1.889611 -1.125683 -0.000246
6 -4.126402 -0.833269 0.000068
1 -5.156296 -1.161331 0.000259
6 -3.592013 0.408416 -0.000164
1 -4.049615 1.387435 -0.000225
6 -3.265257 -3.186290 0.000161
1 -2.284707 -3.665089 0.000397
1 -3.822264 -3.482965 -0.892442
1 -3.822590 -3.482731 0.892637
6 -1.231026 2.522293 0.000130
6 0.000007 3.192702 0.000381
6 1.231036 2.522287 0.000293
6 3.592015 0.408402 -0.000240
1 4.049620 1.387420 -0.000355
6 4.126401 -0.833284 -0.000200
1 5.156294 -1.161349 -0.000258
6 3.265248 -3.186302 0.000203
1 3.822046 -3.482765 0.893007
1 3.822786 -3.482959 -0.892072
1 2.284696 -3.665098 -0.000153
7 0.000001 0.503649 -0.000692
1 -0.000023 -2.863012 0.000510
1 -2.173618 3.059233 0.000366
1 2.173630 3.059224 0.000660
6 0.000010 4.626388 0.000906
7 0.000011 5.787650 0.001304

CN-CNC-0

0 1
28 -0.000080 -1.396155 0.042468
7 -2.215798 0.198062 -0.188956
7 2.215812 0.197823 -0.188942
7 3.100309 -1.736943 0.092521
7 -3.100517 -1.736597 0.092528
6 -1.890386 -1.126540 0.075578
6 -1.158371 1.110991 -0.274606

6 1.158487 1.110867 -0.274596
6 1.890249 -1.126740 0.075602
6 4.137194 -0.839762 -0.122460
1 5.171597 -1.155478 -0.131239
6 3.586051 0.384374 -0.293112
1 4.033719 1.347961 -0.492079
6 3.293633 -3.154110 0.329292
1 2.338242 -3.581580 0.645435
1 4.038788 -3.306211 1.115793
1 3.627757 -3.656538 -0.583732
6 1.221432 2.453915 0.007986
6 0.000166 3.162585 0.076945
6 -1.221176 2.454045 0.007978
6 -3.586019 0.384782 -0.293062
1 -4.033577 1.348427 -0.491996
6 -4.137303 -0.839294 -0.122428
1 -5.171743 -1.154888 -0.131185
6 -3.293996 -3.153752 0.329244
1 -3.628094 -3.656125 -0.583820
1 -4.039228 -3.305799 1.115682
1 -2.338673 -3.581320 0.645461
7 0.000024 0.457119 -0.573315
1 2.170949 2.950455 0.188497
1 -2.170641 2.950686 0.188484
6 0.000230 4.557509 0.323049
7 0.000458 5.709038 0.516613

NMe_2-CNC-II-CO

2 1

28 -1.446850 0.000084 -0.002918
7 0.178221 2.225102 0.023931
7 0.177981 -2.225083 0.022564
7 -1.791895 -3.074486 0.023955
7 -1.791603 3.074598 0.028852
6 -1.151205 1.903704 0.015062
6 1.086061 1.158701 0.021319
6 1.085925 -1.158769 0.022287
6 -1.151422 -1.903594 0.012670
6 -0.884601 -4.125716 0.039641
1 -1.216083 -5.154202 0.050920
6 0.361174 -3.594269 0.038589
1 1.339194 -4.053302 0.049334
6 -3.240265 -3.248158 0.018317
1 -3.676439 -2.762649 0.894657
1 -3.460099 -4.315440 0.058009
1 -3.660597 -2.832943 -0.901036
6 2.449257 -1.226951 0.005541
1 2.942880 -2.191417 -0.007182
6 3.180716 -0.000195 -0.005269
6 2.449386 1.226684 0.003198
1 2.943428 2.191023 -0.004145
6 0.361503 3.594249 0.041729
1 1.339560 4.053212 0.052083
6 -0.884241 4.125764 0.045103
1 -1.215665 5.154244 0.058503
6 -3.239975 3.248240 0.024591
1 -3.660873 2.834872 -0.895342
1 -3.459848 4.315423 0.066666
1 -3.675539 2.760830 0.900171
7 0.407646 0.000003 0.035189

7 4.520402 -0.000131 -0.027852
6 -3.229487 0.000097 -0.089613
8 -4.364496 -0.000018 -0.160136
6 5.257070 -1.257424 -0.023830
1 5.012544 -1.855051 0.862061
1 5.039597 -1.848205 -0.921961
1 6.325179 -1.041275 -0.003984
6 5.255678 1.257349 -0.069211
1 4.990256 1.841544 -0.958356
1 5.058276 1.861230 0.824571
1 6.323289 1.041601 -0.109395

NMe_2-CNC-II-$COOH^-$

1 1
28 -1.305529 0.000182 -0.056197
7 0.336541 -2.218924 -0.037960
7 0.336898 2.219012 -0.037095
7 -1.618454 3.093360 -0.024308
7 -1.618929 -3.093060 -0.028806
6 -1.006174 -1.901917 -0.041375
6 1.256113 -1.154803 -0.043947
6 1.256324 1.154775 -0.044847
6 -1.005858 1.902173 -0.039502
6 -0.699658 4.136123 -0.004648
1 -1.016784 5.169325 0.007972
6 0.537143 3.587285 -0.014454
1 1.520278 4.035835 -0.014770
6 -3.061204 3.289866 0.017028
1 -3.548233 2.506075 -0.565705
1 -3.296043 4.262920 -0.418877
1 -3.416910 3.259681 1.050776
6 2.625293 1.227794 -0.002737
1 3.124691 2.188891 0.029950
6 3.351135 -0.000184 0.009598
6 2.625050 -1.228039 -0.000754
1 3.124496 -2.189263 0.027477
6 0.536600 -3.587252 -0.017227
1 1.519686 -4.035915 -0.017148
6 -0.700270 -4.135961 -0.009824
1 -1.017524 -5.169147 0.000722
6 -3.061723 -3.289602 0.010740
1 -3.418305 -3.262232 1.044266
1 -3.296217 -4.261449 -0.428037
1 -3.548232 -2.504209 -0.570243
7 0.592569 0.000030 -0.083292
7 4.698601 -0.000345 0.040753
6 -3.155117 0.000241 -0.034994
8 -3.681960 -0.000918 1.215584
8 -3.891594 0.000996 -1.007047
1 -4.653784 -0.000987 1.108671
6 5.432440 1.255434 0.041430
1 5.191019 1.858137 -0.842844
1 5.215381 1.848147 0.939333
1 6.501568 1.041717 0.023193
6 5.430869 -1.256394 0.082591
1 5.171487 -1.841729 0.973749
1 5.230612 -1.866042 -0.807556
1 6.499695 -1.043207 0.116768

NMe_2-CNC-II-CO_2^{2-}

0 1

28 1.388303 0.001935 -0.019899

7 -0.310357 -2.216229 0.010181

7 -0.314548 2.216028 -0.057316

7 1.622769 3.124209 0.014504

7 1.629747 -3.120943 0.001989

6 1.044085 -1.909827 0.006762

6 -1.236883 -1.152637 -0.011559

6 -1.239261 1.150626 -0.053245

6 1.040138 1.912106 -0.021995

6 0.689178 4.153740 -0.005252

1 0.986092 5.193195 0.017643

6 -0.536398 3.582609 -0.046368

1 -1.526170 4.016559 -0.062472

6 3.062722 3.332686 0.043406

1 3.526518 2.482056 0.550678

1 3.279189 4.255420 0.587407

1 3.455661 3.415661 -0.975032

6 -2.613802 1.226647 -0.026204

1 -3.120587 2.184711 -0.019878

6 -3.334564 -0.002596 0.001866

6 -2.611248 -1.230470 0.019728

1 -3.115818 -2.188844 0.060546

6 -0.529353 -3.583363 0.015864

1 -1.518419 -4.019217 0.012263

6 0.697988 -4.152232 0.013213

1 0.997373 -5.191232 0.011452

6 3.070474 -3.325933 0.017661

1 3.304479 -4.257250 -0.503977

1 3.434630 -3.390006 1.048118

1 3.546220 -2.482800 -0.490850

7 -0.585155 -0.000872 -0.061978

7 -4.688749 -0.003714 0.019621

6 3.270890 0.001483 0.021653

8 3.789344 -0.217926 -1.090806

8 3.778373 0.217845 1.138373

6 -5.421319 1.250164 0.001759

1 -5.202557 1.859907 0.888487

1 -5.184603 1.841613 -0.892244

1 -6.491158 1.037567 -0.008705

6 -5.418328 -1.258755 0.062803

1 -5.203752 -1.880210 -0.816596

1 -5.174652 -1.837179 0.963653

1 -6.488545 -1.048327 0.076613

NMe_2-CNC-II-$HCOO^-$

1 1

28 1.308970 0.000517 -0.235397

7 -0.317753 2.227769 -0.096279

7 -0.316674 -2.227270 -0.094651

7 1.643373 -3.082902 -0.208526

7 1.642436 3.084099 -0.202332

6 1.013236 1.905991 -0.196472

6 -1.221673 1.157618 -0.052072

6 -1.220936 -1.157515 -0.049019

6 1.013916 -1.904982 -0.198629

6 0.737947 -4.134223 -0.105828

1 1.066572 -5.163962 -0.098660

6 -0.502807 -3.597982 -0.035894

1 -1.478700 -4.055019 0.043686

6 3.088863 -3.253587 -0.269151

1 3.525632 -2.365667 -0.728254

1 3.319320 -4.136183 -0.869673

1 3.491978 -3.383971 0.739649

6 -2.585800 -1.225572 0.043312

1 -3.080064 -2.189251 0.080944

6 -3.314216 -0.000453 0.076581

6 -2.586672 1.225051 0.038531

1 -3.081202 2.188476 0.078371

6 -0.504431 3.598329 -0.035785

1 -1.480688 4.054992 0.041377

6 0.736420 4.134997 -0.100773

1 1.064704 5.164821 -0.090689

6 3.088152 3.255101 -0.256514

1 3.487216 3.380716 0.754504

1 3.320908 4.140585 -0.851867

1 3.526859 2.369451 -0.718136

7 -0.548659 0.000193 -0.108086

7 -4.657977 -0.000883 0.143733

8 3.168619 0.000921 -0.431150

6 3.790349 -0.000663 0.698496

6 -5.392717 1.255124 0.151050

1 -5.158752 1.852056 1.041571

1 -5.167213 1.852022 -0.741126

1 -6.461714 1.040591 0.153314

6 -5.389242 -1.257935 0.194793

1 -5.212096 -1.859141 -0.705794

1 -5.105297 -1.849483 1.073923

1 -6.456627 -1.045190 0.259545

8 3.295908 -0.002542 1.819703

1 4.896242 -0.000197 0.567255

NMe_2-CNC-II-H^-

1 1

28 -1.747707 0.000107 -0.000790

7 -0.118139 2.217905 0.000786

7 -0.118462 -2.217929 -0.001120

7 -2.081055 -3.078427 -0.001654

7 -2.080607 3.078689 0.002322

6 -1.461064 1.891545 0.000878

6 0.804118 1.156389 -0.000326

6 0.803953 -1.156549 -0.000164

6 -1.461339 -1.891372 -0.001485

6 -1.168973 -4.128449 -0.001132

1 -1.493904 -5.159393 -0.001099

6 0.071545 -3.588165 -0.001181

1 1.051351 -4.044218 -0.001043

6 -3.522056 -3.271645 -0.002131

1 -4.001960 -2.291493 -0.002775

1 -3.820645 -3.828210 0.890326

1 -3.819945 -3.829030 -0.894310

6 2.173788 -1.228886 0.000438

1 2.673940 -2.190127 -0.002139

6 2.898965 -0.000226 0.000037

6 2.173961 1.228526 -0.000480

1 2.674266 2.189691 0.002398

6 0.072067 3.588114 0.002187

1 1.051939 4.044025 0.002436

6 -1.168373 4.128579 0.002947

1 -1.493152 5.159570 0.004073

6 -3.521580 3.272118 0.002965

1 -3.820074 3.829624 -0.888936
1 -3.819398 3.828651 0.895699
1 -4.001633 2.292039 0.002601
7 0.141539 -0.000032 -0.000456
7 4.247285 -0.000243 0.000176
1 -3.221657 0.000213 -0.001083
6 4.980599 1.255522 -0.020073
1 4.731445 1.849485 -0.908337
1 4.771212 1.857238 0.873549
1 6.049668 1.042011 -0.044898
6 4.980681 -1.255966 0.020125
1 4.731429 -1.850236 0.908149
1 4.771515 -1.857413 -0.873734
1 6.049728 -1.042377 0.045245

NMe_2-CNC-0

0 1
28 -1.804882 -0.009297 0.044676
7 -0.157787 2.196785 -0.222065
7 -0.133644 -2.196686 -0.227675
7 -2.044166 -3.113933 0.110391
7 -2.081201 3.092247 0.101599
6 -1.492911 1.867264 0.050027
6 0.776236 1.149003 -0.322174
6 0.788911 -1.138985 -0.329296
6 -1.471051 -1.882134 0.050916
6 -1.127867 -4.138212 -0.089212
1 -1.421446 -5.179125 -0.070495
6 0.079680 -3.563943 -0.291372
1 1.050241 -3.996424 -0.491377
6 -3.449536 -3.342388 0.378818
1 -3.895362 -2.390047 0.681373
1 -3.565591 -4.074392 1.184229
1 -3.960993 -3.710786 -0.516224
6 2.145397 -1.208673 -0.085898
1 2.622298 -2.160592 0.122795
6 2.867400 0.015751 -0.035927
6 2.131487 1.232180 -0.074721
1 2.597870 2.188584 0.137288
6 0.039380 3.566354 -0.289714
1 1.005706 4.009699 -0.486567
6 -1.176184 4.126746 -0.096751
1 -1.482227 5.164139 -0.084438
6 -3.491516 3.303734 0.357785
1 -4.000061 3.662956 -0.542653
1 -3.623862 4.036386 1.160058
1 -3.927546 2.346445 0.659094
7 0.143744 0.002235 -0.578878
7 4.217882 0.022488 0.134439
6 4.911722 1.272873 0.375153
1 4.741547 1.983912 -0.442942
1 4.597069 1.748242 1.315713
1 5.984512 1.080098 0.432539
6 4.934273 -1.226265 0.306970
1 4.676638 -1.730011 1.250479
1 4.724474 -1.916047 -0.519501
1 6.007105 -1.024500 0.307366

NO_2-CNC-II-CO

2 1

28 -1.372760 0.000050 -0.001170
7 0.245302 2.225059 0.027047
7 0.245152 -2.225088 0.027708
7 -1.723194 -3.074692 0.029208
7 -1.723037 3.074692 0.029157
6 -1.088601 1.904984 0.017301
6 1.147072 1.167264 0.025725
6 1.147009 -1.167362 0.026027
6 -1.088762 -1.904979 0.017608
6 -0.813073 -4.126125 0.045343
1 -1.144648 -5.154545 0.057455
6 0.431955 -3.596695 0.043617
1 1.411237 -4.053142 0.054920
6 -3.172299 -3.253782 0.022760
1 -3.608685 -2.764689 0.896676
1 -3.387543 -4.321545 0.067781
1 -3.590404 -2.844125 -0.899927
6 2.529020 -1.228164 0.004545
1 3.068410 -2.168670 -0.008610
6 3.174273 -0.000099 -0.005601
6 2.529074 1.227986 0.004464
1 3.068471 2.168477 -0.008742
6 0.432118 3.596665 0.043116
1 1.411402 4.053117 0.054181
6 -0.812905 4.126112 0.044829
1 -1.144447 5.154544 0.056957
6 -3.172168 3.253591 0.022734
1 -3.590066 2.844689 -0.900399
1 -3.387599 4.321272 0.068769
1 -3.608588 2.763417 0.896025
7 0.500400 -0.000027 0.039072
7 4.656348 -0.000051 -0.042351
8 5.210532 1.082394 -0.054595
8 5.210462 -1.082446 -0.060225
6 -3.159174 0.000336 -0.100935
8 -4.292032 0.000322 -0.177730

NO_2-CNC-II-$COOH^-$

1 1
28 1.232190 -0.000073 0.061225
7 -0.401818 -2.220321 0.044311
7 -0.401625 2.220252 0.044531
7 1.553042 3.092588 0.023011
7 1.552815 -3.092753 0.023168
6 0.944663 -1.903166 0.042637
6 -1.315226 -1.165083 0.051175
6 -1.315123 1.165081 0.051290
6 0.944842 1.903010 0.042581
6 0.632660 4.136243 0.005234
1 0.950871 5.169005 -0.010376
6 -0.604015 3.590915 0.020135
1 -1.587947 4.037692 0.022900
6 2.996128 3.293058 -0.023571
1 3.487192 2.510974 0.557747
1 3.228594 4.266735 0.411670
1 3.345357 3.264195 -1.059343
6 -2.699447 1.230941 0.008311
1 -3.244320 2.167683 -0.018241
6 -3.343680 0.000092 -0.006293
6 -2.699561 -1.230814 0.008132

1 -3.244501 -2.167514 -0.018592
6 -0.604262 -3.590976 0.019881
1 -1.588216 -4.037703 0.022389
6 0.632390 -4.136376 0.005362
1 0.950573 -5.169147 -0.010164
6 2.995947 -3.293015 -0.023368
1 3.345371 -3.262545 -1.059024
1 3.228427 -4.267320 0.410445
1 3.486802 -2.511681 0.559156
7 -0.679762 -0.000032 0.086071
7 -4.822513 0.000173 -0.058590
8 -5.381333 -1.081239 -0.079330
8 -5.381236 1.081649 -0.078766
6 3.079163 -0.000094 0.033530
8 3.592467 0.000211 -1.218032
8 3.808421 -0.000221 1.008007
1 4.566065 0.000224 -1.125628

NO_2-CNC-II-CO_2^{2-}

0 1
28 1.304779 0.001152 0.076127
7 -0.378585 2.221957 0.082395
7 -0.374899 -2.214245 0.149899
7 1.558145 -3.113816 -0.037902
7 1.560880 3.120585 -0.012903
6 0.973325 1.912541 -0.004637
6 -1.292630 1.164706 0.127092
6 -1.291447 -1.158502 0.169995
6 0.973673 -1.904577 0.011506
6 0.631696 -4.146756 0.061350
1 0.933398 -5.184720 0.037578
6 -0.591956 -3.584126 0.171507
1 -1.576640 -4.019866 0.263586
6 2.992548 -3.323557 -0.165693
1 3.423188 -2.480507 -0.712092
1 3.169920 -4.250683 -0.715937
1 3.456148 -3.397003 0.822873
6 -2.670053 -1.230697 0.040184
1 -3.212317 -2.167531 -0.021402
6 -3.321314 -0.001211 -0.020722
6 -2.671128 1.230174 -0.008168
1 -3.214174 2.163375 -0.107257
6 -0.595780 3.592210 0.102516
1 -1.582235 4.028028 0.171998
6 0.631932 4.154382 0.044380
1 0.935203 5.192191 0.043918
6 2.999363 3.320407 -0.115202
1 3.260901 4.271482 0.354140
1 3.308012 3.337714 -1.165126
1 3.502644 2.501760 0.404348
7 -0.659930 0.005689 0.276716
7 -4.784282 -0.004701 -0.151393
8 -5.348554 1.075016 -0.230906
8 -5.348552 -1.087184 -0.170260
6 3.179156 -0.008778 -0.154753
8 3.603173 0.132578 1.006712
8 3.709999 -0.149418 -1.257043

NO_2-CNC-II-$HCOO^-$

1 1

28 1.237010 0.000202 -0.241043
7 -0.379396 2.228754 -0.106901
7 -0.379079 -2.228633 -0.107036
7 1.582601 -3.079870 -0.206121
7 1.582295 3.080009 -0.206137
6 0.955066 1.905197 -0.203980
6 -1.276850 1.167469 -0.062208
6 -1.276659 -1.167442 -0.062295
6 0.955373 -1.905062 -0.204281
6 0.676108 -4.133072 -0.105771
1 1.007264 -5.161897 -0.093802
6 -0.565668 -3.601985 -0.044702
1 -1.542070 -4.058739 0.029625
6 3.029252 -3.253163 -0.256435
1 3.470827 -2.369213 -0.718089
1 3.260063 -4.140144 -0.849875
1 3.422073 -3.378631 0.756798
6 -2.657268 -1.228066 0.034935
1 -3.196785 -2.167516 0.076567
6 -3.302409 -0.000150 0.074019
6 -2.657461 1.227871 0.035022
1 -3.197123 2.167235 0.076758
6 -0.566005 3.602118 -0.045045
1 -1.542411 4.058884 0.029139
6 0.675765 4.133217 -0.106113
1 1.006877 5.162057 -0.094455
6 3.028980 3.253114 -0.256027
1 3.421579 3.378140 0.757349
1 3.260068 4.140313 -0.849033
1 3.470546 2.369289 -0.717937
7 -0.631874 0.000059 -0.119737
7 -4.779018 -0.000272 0.169717
8 -5.335716 1.081418 0.205560
8 -5.335567 -1.082058 0.204992
8 3.089825 -0.000031 -0.418891
6 3.682050 -0.000111 0.728973
8 3.151797 0.000022 1.832801
1 4.789739 -0.000193 0.627413

NO_2-CNC-II-H^-

1 1
28 -1.665583 0.000022 -0.000926
7 -0.047702 2.218957 -0.000395
7 -0.047761 -2.218960 -0.000152
7 -2.011941 -3.073548 -0.003785
7 -2.011852 3.073601 0.004657
6 -1.394034 1.889781 0.000930
6 0.869654 1.167093 -0.001693
6 0.869623 -1.167121 0.000858
6 -1.394084 -1.889744 -0.001574
6 -1.100508 -4.126409 -0.003882
1 -1.428633 -5.156271 -0.005633
6 0.141087 -3.592195 -0.001595
1 1.120274 -4.049425 -0.001048
6 -3.453971 -3.265891 -0.006440
1 -3.933160 -2.285552 -0.004855
1 -3.751313 -3.825328 0.884383
1 -3.748630 -3.821174 -0.900757
6 2.254685 -1.231879 0.003576
1 2.801568 -2.167712 0.006639

6 2.898131 -0.000039 -0.000074
6 2.254718 1.231817 -0.003871
1 2.801621 2.167639 -0.006581
6 0.141191 3.592183 0.002617
1 1.120393 4.049381 0.002455
6 -1.100386 4.126433 0.005728
1 -1.428480 5.156303 0.008705
6 -3.453876 3.265987 0.007798
1 -3.751340 3.826568 -0.882264
1 -3.748373 3.820144 0.902868
1 -3.933098 2.285668 0.005023
7 0.235478 -0.000006 -0.000662
7 4.377569 -0.000052 0.000199
8 4.937227 1.079927 -0.054976
8 4.937188 -1.080043 0.055566
1 -3.129747 0.000042 -0.001034

NO_2-CNC-0

0 1
28 -1.642898 0.000008 0.036636
7 -0.067891 2.223873 -0.193207
7 -0.067912 -2.223874 -0.193193
7 -2.003287 -3.100157 0.099324
7 -2.003253 3.100177 0.099326
6 -1.384035 1.899629 0.067743
6 0.841158 1.160595 -0.285863
6 0.841147 -1.160605 -0.285855
6 -1.384054 -1.899616 0.067753
6 -1.110150 -4.141192 -0.110869
1 -1.429463 -5.174392 -0.109320
6 0.115348 -3.593804 -0.290754
1 1.077623 -4.044575 -0.488492
6 -3.422547 -3.283337 0.337544
1 -3.850961 -2.319243 0.622556
1 -3.577632 -4.003200 1.146319
1 -3.919633 -3.645894 -0.567175
6 2.181179 -1.223450 -0.029815
1 2.690466 -2.166763 0.137693
6 2.887971 -0.000014 0.021789
6 2.181191 1.223429 -0.029826
1 2.690487 2.166738 0.137675
6 0.115384 3.593801 -0.290768
1 1.077663 4.044561 -0.488516
6 -1.110102 4.141204 -0.110845
1 -1.429400 5.174409 -0.109276
6 -3.422511 3.283374 0.337546
1 -3.919593 3.645940 -0.567172
1 -3.577586 4.003238 1.146322
1 -3.850937 2.319285 0.622555
7 0.169695 -0.000003 -0.583437
7 4.277071 -0.000020 0.224442
8 4.869336 1.091973 0.308219
8 4.869325 -1.092019 0.308226

OMe-CNC-II-CO

2 1
28 1.177531 0.277608 0.000556
7 0.218464 -2.305311 0.000741
7 -0.989407 1.977185 0.002791
7 0.676663 3.327416 0.004362

7 2.342594 -2.596967 0.005524
6 1.414478 -1.638831 0.002605
6 -0.941808 -1.528930 0.000795
6 -1.571302 0.707408 0.001846
6 0.378731 2.028367 0.002277
6 -0.482043 4.094103 0.006277
1 -0.439373 5.174027 0.008520
6 -1.537762 3.246790 0.005182
1 -2.603540 3.424973 0.006292
6 2.023790 3.888122 0.004969
1 2.560967 3.560853 0.898408
1 1.943833 4.975398 0.017122
1 2.554530 3.580378 -0.899316
6 -2.912211 0.400759 -0.000709
1 -3.661599 1.184503 -0.002084
6 -3.246674 -0.967314 -0.002227
6 -2.241219 -1.958385 -0.001340
1 -2.506430 -3.010465 -0.003171
6 0.405702 -3.673949 0.001903
1 -0.415415 -4.376621 0.001251
6 1.747700 -3.852487 0.004776
1 2.342837 -4.754535 0.006857
6 3.786455 -2.382670 0.007489
1 4.086299 -1.863090 -0.905997
1 4.278248 -3.355342 0.041233
1 4.074220 -1.808547 0.891558
7 -0.615937 -0.227565 0.003070
6 2.897984 0.762215 -0.013391
8 3.992222 1.068954 -0.026535
8 -4.486946 -1.417760 -0.005027
6 -5.570107 -0.481965 -0.006714
1 -5.544438 0.142005 0.893482
1 -5.540132 0.143674 -0.905612
1 -6.480012 -1.082485 -0.009440

OMe-CNC-II-COOH$^-$

1 1
28 -1.059895 0.153539 -0.033385
7 0.124886 -2.340073 -0.015689
7 0.975238 2.016475 -0.019543
7 -0.775998 3.248410 -0.035170
7 -1.961068 -2.823077 -0.031034
6 -1.133176 -1.771342 -0.024486
6 1.229667 -1.476066 -0.018321
6 1.671231 0.798792 -0.020243
6 -0.404511 1.962823 -0.027430
6 0.326043 4.096363 -0.023331
1 0.211366 5.171098 -0.027004
6 1.435032 3.322042 -0.015441
1 2.485392 3.575348 -0.014376
6 -2.155286 3.717849 -0.020172
1 -2.768798 3.050886 -0.628852
1 -2.187332 4.724717 -0.440348
1 -2.534604 3.740340 1.005250
6 3.039001 0.608861 0.001873
1 3.723531 1.449865 0.013101
6 3.480065 -0.727455 0.011883
6 2.564285 -1.800840 0.002745
1 2.922211 -2.825137 0.017842
6 0.060035 -3.722131 -0.010355

1 0.939125 -4.350608 -0.008258
6 -1.258898 -4.023081 -0.017887
1 -1.769412 -4.975720 -0.020730
6 -3.415332 -2.738647 -0.013584
1 -3.775529 -2.643572 1.014665
1 -3.825710 -3.646969 -0.458776
1 -3.731966 -1.873895 -0.599435
7 0.809968 -0.210830 -0.037173
6 -2.875562 0.510215 -0.042188
8 -3.408791 0.616374 1.199340
8 -3.579565 0.646267 -1.027628
1 -4.361951 0.800944 1.082420
8 4.760259 -1.077601 0.036660
6 5.754299 -0.054046 0.064536
1 5.706718 0.562033 -0.840793
1 5.642241 0.575316 0.954620
1 6.714007 -0.570421 0.103144

OMe-CNC-II-CO_2^{2-}

0 1
28 -1.138278 0.191604 -0.002578
7 0.990697 2.002002 0.020733
7 0.057331 -2.331778 -0.057404
7 -2.027187 -2.811403 0.000984
7 -0.712454 3.297396 -0.009465
6 -0.399792 1.990117 0.011464
6 1.668859 0.769643 0.002662
6 1.184201 -1.490287 -0.046459
6 -1.203691 -1.748712 -0.021987
6 -1.330960 -4.014554 -0.025803
1 -1.841439 -4.967565 -0.012652
6 -0.012581 -3.715028 -0.059086
1 0.864050 -4.347025 -0.076207
6 -3.479351 -2.713418 0.025619
1 -3.756751 -1.801870 0.562091
1 -3.886578 -3.588379 0.537780
1 -3.874578 -2.676954 -0.994532
6 2.515553 -1.846071 -0.039742
1 2.860107 -2.875220 -0.053200
6 3.449417 -0.789690 -0.005085
6 3.038364 0.555202 0.018635
1 3.744034 1.378258 0.048980
6 1.495956 3.292254 0.011175
1 2.554569 3.509750 0.007446
6 0.417500 4.107432 -0.005219
1 0.344938 5.186144 -0.020885
6 -2.075006 3.808716 -0.011065
1 -2.102241 4.749980 -0.565388
1 -2.415971 3.985408 1.014016
1 -2.720930 3.071482 -0.495660
7 0.798513 -0.221938 -0.030594
6 -2.981877 0.577699 0.032028
8 -3.442137 0.914557 -1.074525
8 -3.514264 0.448328 1.149544
8 4.728169 -1.168651 0.006989
6 5.737687 -0.166938 0.069247
1 5.703506 0.485168 -0.811787
1 5.641459 0.433750 0.981408
1 6.689472 -0.699874 0.086629

OMe-CNC-II-HCOO$^-$

1 1

28 1.061571 0.182342 -0.224760

7 -1.010789 2.000606 -0.117524

7 -0.037383 -2.347031 -0.101498

7 2.061759 -2.754050 -0.205690

7 0.714094 3.264367 -0.222322

6 0.361279 1.978214 -0.197267

6 -1.655389 0.762278 -0.057310

6 -1.151080 -1.504323 -0.052107

6 1.192570 -1.741549 -0.196055

6 1.406088 -3.978150 -0.114285

1 1.952384 -4.910831 -0.108976

6 0.078257 -3.726328 -0.049429

1 -0.775157 -4.385075 0.023222

6 3.510611 -2.609266 -0.254817

1 3.748669 -1.636528 -0.687131

1 3.927873 -3.405990 -0.874250

1 3.925272 -2.677897 0.755194

6 -2.472655 -1.859133 0.049357

1 -2.796554 -2.893743 0.093683

6 -3.417074 -0.813724 0.104068

6 -3.010813 0.531640 0.050757

1 -3.712565 1.357175 0.094679

6 -1.496386 3.298357 -0.090208

1 -2.550320 3.530541 -0.035645

6 -0.402856 4.092172 -0.154808

1 -0.307746 5.168861 -0.165442

6 2.087115 3.749412 -0.267334

1 2.440713 3.960170 0.746330

1 2.122794 4.663606 -0.863368

1 2.712548 2.981008 -0.723867

7 -0.757495 -0.224035 -0.107075

8 2.873863 0.588486 -0.414765

6 3.470766 0.733304 0.719569

8 -4.681227 -1.196498 0.211037

6 -5.699075 -0.198388 0.295050

1 -5.546444 0.439390 1.172701

1 -5.723837 0.411995 -0.614914

1 -6.640471 -0.739306 0.396223

8 2.975982 0.631819 1.835739

1 4.550457 0.974506 0.596455

OMe-CNC-II-H$^-$

1 1

28 1.050022 1.076418 -0.000707

7 1.609312 -1.617825 -0.000138

7 -1.686228 1.351718 0.000300

7 -1.014641 3.385563 0.000269

7 3.561294 -0.735239 0.000143

6 2.265635 -0.400286 -0.000667

6 0.206801 -1.595208 -0.000201

6 -1.514794 -0.039707 0.000143

6 -0.544416 2.132952 0.000092

6 -2.405979 3.408522 0.000608

1 -2.955381 4.339378 0.000837

6 -2.833706 2.125562 0.000604

1 -3.827421 1.700763 0.000828

6 -0.198618 4.589084 0.000193

1 0.852344 4.295453 0.000058

1 -0.416611 5.182097 0.892402
1 -0.416822 5.182144 -0.891935
6 -2.493828 -1.014029 0.000093
1 -3.545394 -0.749777 0.000270
6 -2.043208 -2.347380 -0.000255
6 -0.666055 -2.656476 -0.000455
1 -0.338919 -3.690988 -0.000811
6 2.500546 -2.677047 0.001111
1 2.184988 -3.710469 0.001808
6 3.731130 -2.115875 0.001197
1 4.715426 -2.562957 0.001908
6 4.672497 0.202818 -0.000055
1 5.285755 0.046374 -0.891409
1 5.283606 0.049419 0.893307
1 4.269515 1.217029 -0.002276
7 -0.219434 -0.331550 0.000033
1 2.033192 2.169155 -0.001459
8 -2.856978 -3.396939 -0.000337
6 -4.266330 -3.175831 0.000003
1 -4.576909 -2.629065 0.897824
1 -4.577305 -2.628935 -0.897607
1 -4.725027 -4.165083 0.000026

OMe-CNC-0

0 1
28 0.964035 1.225497 0.048133
7 1.770570 -1.411069 -0.181700
7 -1.791099 1.172312 -0.203786
7 -1.390766 3.263961 0.064710
7 3.630701 -0.376867 0.094647
6 2.294063 -0.134093 0.065544
6 0.375530 -1.547511 -0.261354
6 -1.484178 -0.194916 -0.272857
6 -0.742508 2.069695 0.047424
6 -2.759392 3.130304 -0.130881
1 -3.421153 3.986036 -0.139363
6 -3.017802 1.812442 -0.288932
1 -3.942816 1.283809 -0.472590
6 -0.737069 4.536702 0.294385
1 0.294763 4.338052 0.598725
1 -1.253934 5.089047 1.085242
1 -0.731610 5.140018 -0.619021
6 -2.348374 -1.251153 -0.020046
1 -3.404967 -1.082309 0.159786
6 -1.765604 -2.527347 0.053877
6 -0.366573 -2.683011 -0.007797
1 0.082483 -3.653747 0.182215
6 2.761883 -2.377096 -0.254632
1 2.548436 -3.422015 -0.431979
6 3.932329 -1.719990 -0.091966
1 4.951448 -2.082264 -0.092334
6 4.632589 0.646834 0.314365
1 5.180274 0.859211 -0.609447
1 5.340361 0.321951 1.083145
1 4.120430 1.555205 0.645608
7 -0.184506 -0.359392 -0.513590
8 -2.461386 -3.652591 0.271544
6 -3.873138 -3.558013 0.387593
1 -4.237729 -4.578959 0.514754
1 -4.163218 -2.961203 1.261587

1 -4.319517 -3.125733 -0.516703

TS-CN-CNC-II-H-CO_2

1 1

28 -0.919416 0.000001 -0.074886

7 0.688971 -2.226674 -0.058499

7 0.938645 -0.000001 -0.049253

7 0.688975 2.226673 -0.058499

7 -1.281257 3.067725 -0.111455

7 -1.281263 -3.067722 -0.111455

6 -0.644425 -1.897315 -0.101457

6 1.588986 -1.168103 -0.031191

6 1.588988 1.168100 -0.031190

6 -0.644421 1.897316 -0.101456

6 -0.375413 4.125258 -0.071224

1 -0.711072 5.152577 -0.075335

6 0.870438 3.601530 -0.039049

1 1.846540 4.063809 -0.011550

6 -2.728727 3.240996 -0.113214

1 -2.964830 4.200658 -0.576283

1 -3.108318 3.225211 0.911789

1 -3.190778 2.439019 -0.692033

6 2.969745 1.226190 0.014474

6 3.644187 -0.000003 0.037734

6 2.969742 -1.226195 0.014473

6 0.870432 -3.601531 -0.039048

1 1.846533 -4.063812 -0.011549

6 -0.375420 -4.125257 -0.071223

1 -0.711081 -5.152575 -0.075333

6 -2.728733 -3.240991 -0.113215

1 -3.108325 -3.225205 0.911788

1 -2.964837 -4.200652 -0.576284

1 -3.190783 -2.439013 -0.692033

6 -3.271773 0.000002 0.135678

8 -2.736189 0.000003 1.263169

8 -4.425164 -0.000001 -0.258558

1 -2.500956 0.000004 -0.799994

1 3.499261 2.172920 0.032168

1 3.499257 -2.172927 0.032167

6 5.076300 -0.000004 0.090203

7 6.236560 -0.000005 0.132109

TS-NMe_2-CNC-II-H-CO_2

1 1

28 -1.254194 0.000449 -0.071705

7 0.364268 -2.225405 -0.061705

7 0.595409 0.000086 -0.051120

7 0.365192 2.225654 -0.061925

7 -1.603674 3.071772 -0.105327

7 -1.604840 -3.070679 -0.110264

6 -0.966684 -1.897287 -0.097808

6 1.270226 -1.159417 -0.037089

6 1.270754 1.159296 -0.039055

6 -0.965959 1.898112 -0.096027

6 -0.697325 4.127011 -0.072666

1 -1.030071 5.155321 -0.076611

6 0.547789 3.597838 -0.046755

1 1.524516 4.059229 -0.025633

6 -3.050258 3.244677 -0.096024

1 -3.291956 4.201585 -0.562399

1 -3.423659 3.234262 0.931501
1 -3.517892 2.439368 -0.665906
6 2.637500 1.224709 -0.004703
1 3.131925 2.188961 0.006228
6 3.366368 -0.000467 0.018327
6 2.636899 -1.225368 -0.001175
1 3.131137 -2.189775 0.006746
6 0.546301 -3.597687 -0.048411
1 1.522811 -4.059495 -0.026308
6 -0.698968 -4.126326 -0.077579
1 -1.032109 -5.154497 -0.083902
6 -3.051501 -3.243049 -0.104167
1 -3.426873 -3.234781 0.922668
1 -3.292672 -4.198807 -0.573170
1 -3.517761 -2.436254 -0.673068
6 -3.626927 -0.000079 0.128842
8 -3.108861 0.000050 1.264512
8 -4.779692 -0.001397 -0.275044
1 -2.850047 0.001451 -0.792681
7 4.710427 -0.000933 0.055756
6 5.445004 1.255513 0.059813
1 5.212123 1.854461 -0.828924
1 5.217568 1.849264 0.954108
1 6.513922 1.041025 0.053080
6 5.442429 -1.258084 0.101756
1 5.169654 -1.845512 0.987153
1 5.253459 -1.862628 -0.793981
1 6.510448 -1.044805 0.151504

TS-NO_2-CNC-II-H-CO_2

1 1
28 -1.180390 -0.000003 -0.076174
7 0.427975 -2.226845 -0.068145
7 0.677213 0.000000 -0.060028
7 0.427970 2.226843 -0.068146
7 -1.542493 3.067714 -0.110661
7 -1.542486 -3.067720 -0.110655
6 -0.906126 -1.897529 -0.104436
6 1.326611 -1.168791 -0.044401
6 1.326608 1.168792 -0.044400
6 -0.906131 1.897524 -0.104443
6 -0.636117 4.125312 -0.074892
1 -0.971840 5.152614 -0.077127
6 0.609834 3.601927 -0.049243
1 1.586210 4.063911 -0.026643
6 -2.990023 3.241484 -0.105178
1 -3.227933 4.201426 -0.566681
1 -3.364245 3.225455 0.921768
1 -3.455053 2.439893 -0.682132
6 2.708901 1.227448 -0.002392
1 3.248467 2.167677 0.014898
6 3.355859 0.000003 0.018606
6 2.708905 -1.227443 -0.002395
1 3.248473 -2.167670 0.014894
6 0.609843 -3.601929 -0.049249
1 1.586219 -4.063911 -0.026655
6 -0.636108 -4.125316 -0.074893
1 -0.971828 -5.152619 -0.077130
6 -2.990016 -3.241492 -0.105163
1 -3.364232 -3.225460 0.921786

1 -3.227928 -4.201435 -0.566661
1 -3.455050 -2.439903 -0.682116
6 -3.528911 0.000001 0.145268
8 -2.987518 0.000001 1.269923
8 -4.683542 0.000008 -0.244278
1 -2.761836 -0.000006 -0.794925
7 4.833842 0.000006 0.074234
8 5.391069 -1.081806 0.096322
8 5.391062 1.081820 0.096368

TS-OMe-CNC-II-H-CO_2

1 1
28 1.010650 0.123479 -0.066910
7 -0.964318 2.037361 -0.045031
7 -0.816196 -0.194545 -0.023069
7 -0.197461 -2.347619 -0.037682
7 1.886377 -2.841810 -0.104468
7 0.829668 3.207807 -0.102767
6 0.404175 1.943339 -0.084815
6 -1.669607 0.833769 -0.019137
6 -1.271508 -1.457051 -0.013165
6 1.057632 -1.795682 -0.091006
6 1.175457 -4.037353 -0.056116
1 1.681954 -4.992104 -0.060253
6 -0.141685 -3.731373 -0.015396
1 -1.024187 -4.353676 0.020674
6 3.341306 -2.761805 -0.121607
1 3.737084 -3.674998 -0.569445
1 3.724088 -2.658665 0.897308
1 3.650609 -1.903452 -0.721493
6 -2.611330 -1.748711 0.012485
1 -2.982149 -2.768598 0.021698
6 -3.508601 -0.661037 0.025524
6 -3.037000 0.663946 0.005187
1 -3.699911 1.522216 0.005799
6 -1.381058 3.358694 -0.031988
1 -2.421912 3.646763 -0.004990
6 -0.245069 4.092122 -0.066894
1 -0.091489 5.161972 -0.075111
6 2.225702 3.625959 -0.119337
1 2.621254 3.657651 0.899314
1 2.287928 4.619775 -0.566111
1 2.807770 2.924168 -0.720387
6 3.346369 0.533105 0.106912
8 2.846318 0.454604 1.247429
8 4.477787 0.713410 -0.313741
1 2.566401 0.409912 -0.807416
8 -4.792737 -0.983375 0.053839
6 -5.766789 0.061796 0.071650
1 -5.706456 0.664702 -0.841360
1 -6.736185 -0.434916 0.118120
1 -5.638375 0.698049 0.954251

TS-CCC-I-CO_2

0 2
28 -0.000007 -0.573611 -0.191208
7 2.277755 1.060318 -0.032638
7 -2.277636 1.060454 -0.032560
7 -3.143616 -0.889740 -0.232618
7 3.143561 -0.889958 -0.232643

6 1.942528 -0.273186 -0.174085

6 1.194335 1.990995 0.055886

6 -1.194156 1.991063 0.055933

6 -1.942525 -0.273088 -0.173976

6 -4.193011 0.010244 -0.126286

1 -5.225774 -0.309252 -0.153529

6 -3.642256 1.244628 -0.003061

1 -4.100667 2.218910 0.094577

6 -3.318902 -2.327067 -0.341569

1 -2.447772 -2.752802 -0.844791

1 -4.215710 -2.542253 -0.927967

1 -3.421265 -2.779679 0.650502

6 -1.232149 3.380097 0.154855

1 -2.163928 3.942402 0.188271

6 0.000150 4.049233 0.205537

1 0.000183 5.134581 0.282314

6 1.232410 3.380027 0.154799

1 2.164222 3.942280 0.188170

6 3.642395 1.244355 -0.003046

1 4.100898 2.218590 0.094638

6 4.193041 0.009916 -0.126232

1 5.225777 -0.309676 -0.153411

6 3.318584 -2.327303 -0.341645

1 3.421713 -2.779892 0.650358

1 4.214818 -2.542712 -0.928842

1 2.446879 -2.752756 -0.844088

6 -0.000136 -2.935190 0.613841

8 -0.000348 -3.549691 -0.398558

8 0.000115 -2.684662 1.768802

6 0.000068 1.312055 0.017194

TS-CN-CCC-I-CO_2

0 2

28 0.985430 0.000000 -0.277213

7 -0.649899 2.278346 -0.156509

7 -0.649899 -2.278346 -0.156509

7 1.307591 -3.146584 -0.203812

7 1.307591 3.146584 -0.203812

6 0.690736 1.945755 -0.215543

6 -1.579732 1.198201 -0.132989

6 -1.579732 -1.198201 -0.132989

6 0.690736 -1.945755 -0.215543

6 0.400927 -4.193465 -0.127747

1 0.720737 -5.226275 -0.109382

6 -0.838131 -3.642636 -0.097575

1 -1.817402 -4.098233 -0.052268

6 2.749106 -3.327226 -0.193476

1 3.219141 -2.476676 -0.691295

1 3.004749 -4.244507 -0.729575

1 3.118967 -3.396454 0.835012

6 -2.953015 -1.242390 0.054528

1 -3.516395 -2.167730 0.156390

6 -3.620543 0.000000 0.126211

6 -2.953015 1.242390 0.054528

1 -3.516395 2.167729 0.156390

6 -0.838131 3.642636 -0.097575

1 -1.817403 4.098233 -0.052268

6 0.400927 4.193465 -0.127747

1 0.720737 5.226275 -0.109382

6 2.749106 3.327226 -0.193476

1 3.118967 3.396452 0.835012

1 3.004748 4.244508 -0.729572

1 3.219140 2.476677 -0.691297

6 3.174222 0.000000 0.772773

8 3.831774 0.000000 -0.215283

8 2.892496 0.000000 1.920933

6 -0.911941 0.000000 -0.266353

6 -5.035116 0.000000 0.311316

7 -6.190273 0.000000 0.461918

TS-NMe$_2$-CCC-I-CO$_2$

0 2

28 -1.342551 0.002569 -0.386998

7 0.298821 -2.267850 -0.311775

7 0.307986 2.266576 -0.312817

7 -1.643273 3.146445 -0.201865

7 -1.656266 -3.140197 -0.209229

6 -1.042595 -1.938666 -0.295742

6 1.227503 -1.180514 -0.366171

6 1.232407 1.175654 -0.368951

6 -1.034755 1.942691 -0.294132

6 -0.726696 4.186348 -0.148344

1 -1.037388 5.219722 -0.075797

6 0.507630 3.626730 -0.216036

1 1.490938 4.076149 -0.219569

6 -3.078340 3.328546 -0.079205

1 -3.585548 2.478642 -0.540563

1 -3.376529 4.247375 -0.590717

1 -3.369269 3.393209 0.975073

6 2.592754 1.223528 -0.088331

1 3.096136 2.168190 0.098762

6 3.298757 -0.006301 -0.003404

6 2.587162 -1.233356 -0.083581

1 3.087486 -2.179835 0.102684

6 0.492706 -3.629158 -0.219247

1 1.474205 -4.082534 -0.222090

6 -0.744066 -4.184004 -0.156838

1 -1.059098 -5.216378 -0.089062

6 -3.092511 -3.316465 -0.092040

1 -3.387960 -3.378998 0.961112

1 -3.392164 -4.234600 -0.603935

1 -3.594618 -2.465068 -0.556214

6 -3.356064 0.004008 1.073912

8 -4.152542 0.005298 0.197199

8 -2.882620 0.003277 2.154910

6 0.554522 -0.001222 -0.598915

7 4.669704 -0.010402 0.197030

6 5.324351 -1.244158 0.575573

1 5.204315 -2.013279 -0.198374

1 6.395341 -1.060469 0.689431

1 4.945473 -1.658019 1.524647

6 5.344216 1.230728 0.508434

1 5.189554 1.974352 -0.283455

1 5.012012 1.676717 1.460827

1 6.419155 1.045954 0.575015

TS-NO$_2$-CCC-I-CO$_2$

0 2

28 1.262919 -0.000005 -0.341261

7 -0.370142 2.276855 -0.235333

7 -0.370154 -2.276857 -0.235321
7 1.588648 -3.142878 -0.207398
7 1.588666 3.142864 -0.207401
6 0.970193 1.944179 -0.251717
6 -1.296855 1.196773 -0.246035
6 -1.296861 -1.196771 -0.246026
6 0.970183 -1.944188 -0.251711
6 0.680476 -4.189933 -0.149387
1 1.000656 -5.222083 -0.111097
6 -0.559487 -3.640997 -0.164494
1 -1.539470 -4.096878 -0.146753
6 3.029438 -3.320047 -0.143168
1 3.515784 -2.481448 -0.645216
1 3.303725 -4.249822 -0.647429
1 3.363952 -3.363234 0.898827
6 -2.660122 -1.241203 -0.007514
1 -3.222577 -2.160282 0.128292
6 -3.311122 0.000007 0.072792
6 -2.660115 1.241214 -0.007524
1 -3.222567 2.160296 0.128275
6 -0.559468 3.640996 -0.164508
1 -1.539447 4.096883 -0.146772
6 0.680499 4.189925 -0.149396
1 1.000686 5.222073 -0.111105
6 3.029456 3.320024 -0.143155
1 3.363952 3.363248 0.898844
1 3.303759 4.249778 -0.647447
1 3.515807 2.481403 -0.645163
6 3.263143 0.000009 0.939145
8 3.986111 -0.000018 -0.003815
8 2.909584 0.000031 2.066807
6 -0.631315 -0.000002 -0.442024
7 -4.743886 0.000012 0.302656
8 -5.319486 -1.080090 0.394130
8 -5.319480 1.080116 0.394123

TS-OMe-CCC-I-CO_2

0 2
28 1.071663 0.163511 -0.274605
7 -1.000753 2.057385 -0.170100
7 -0.080852 -2.397257 -0.159015
7 2.012123 -2.854586 -0.200023
7 0.735738 3.310860 -0.229543
6 0.380102 2.006854 -0.224409
6 -1.689384 0.804049 -0.146295
6 -1.211060 -1.522897 -0.142603
6 1.166171 -1.800962 -0.215992
6 1.334740 -4.062830 -0.124996
1 1.856338 -5.009881 -0.102952
6 0.009891 -3.770654 -0.099026
1 -0.857781 -4.414102 -0.054400
6 3.459413 -2.738591 -0.182595
1 3.747313 -1.805536 -0.672023
1 3.900093 -3.580141 -0.722837
1 3.831947 -2.738005 0.847377
6 -2.549360 -1.840495 0.040985
1 -2.928102 -2.855569 0.145529
6 -3.461603 -0.766646 0.112364
6 -3.054158 0.577490 0.040371
1 -3.768717 1.390309 0.140670

6 -1.465469 3.353594 -0.131460
1 -2.518082 3.597468 -0.092402
6 -0.366953 4.149731 -0.168558
1 -0.266701 5.226493 -0.163381
6 2.109714 3.780707 -0.226789
1 2.474533 3.898431 0.799464
1 2.166385 4.743328 -0.740665
1 2.735120 3.055058 -0.751466
6 3.293018 0.651320 0.797826
8 3.942436 0.793169 -0.181738
8 2.981018 0.582080 1.934283
6 -0.786986 -0.219738 -0.273779
6 -5.729382 -0.127103 0.408592
1 -5.779957 0.506879 -0.487798
1 -6.689657 -0.632132 0.537713
1 -5.540940 0.508536 1.284922
8 -4.756494 -1.141153 0.278718

CCC-III-H_2O-$OCHO^-$

1 2
28 0.003242 -0.451223 -0.153165
7 -2.310812 1.188385 -0.092905
7 2.269148 1.258076 -0.095290
7 3.108667 -0.714739 -0.207629
7 -3.091846 -0.806722 -0.215600
6 -1.945189 -0.118217 -0.206224
6 -1.236760 2.103572 -0.029855
6 1.167215 2.141445 -0.033731
6 1.941311 -0.060547 -0.187630
6 4.164333 0.181665 -0.129724
1 5.191358 -0.155265 -0.137804
6 3.635345 1.430789 -0.059779
1 4.104231 2.402051 0.004794
6 3.259562 -2.164418 -0.245735
1 3.009295 -2.590392 0.730651
1 4.296520 -2.399433 -0.490800
1 2.598588 -2.583564 -1.006363
6 1.169373 3.529641 0.040218
1 2.098860 4.093084 0.061858
6 -0.066762 4.180658 0.081629
1 -0.083714 5.265833 0.139293
6 -1.281865 3.490910 0.045416
1 -2.228171 4.025270 0.071429
6 -3.681384 1.319631 -0.032165
1 -4.177743 2.275630 0.051835
6 -4.173482 0.056475 -0.109112
1 -5.189753 -0.311838 -0.106362
6 -3.201747 -2.259037 -0.266203
1 -2.477618 -2.655488 -0.979716
1 -4.212385 -2.521460 -0.583541
1 -3.009084 -2.682980 0.724115
6 0.048049 -3.129121 0.431975
8 0.097309 -4.422240 0.117136
8 0.043030 -2.359127 -0.574545
1 0.120997 -4.511121 -0.860498
1 -0.002914 -1.942616 1.707241
8 -0.060659 -0.936725 1.892109
1 0.764920 -0.691052 2.333056
6 -0.024280 1.444439 -0.060450

CNC-II-H_2O-$OCHO^-$

1 1

28 -0.005494 -0.462019 -0.277627

7 -2.240063 1.144324 -0.119826

7 2.218496 1.163689 -0.131551

7 3.085747 -0.781768 -0.348662

7 -3.092600 -0.807990 -0.330531

6 -1.915821 -0.181380 -0.276701

6 -1.178534 2.046944 -0.030712

6 1.149353 2.057819 -0.037740

6 1.903794 -0.165081 -0.283380

6 4.132368 0.129025 -0.235629

1 5.164230 -0.191201 -0.269298

6 3.589672 1.360928 -0.101181

1 4.040319 2.337165 0.004793

6 3.271622 -2.221251 -0.479690

1 3.390663 -2.675111 0.508828

1 4.166237 -2.409791 -1.076701

1 2.398502 -2.647545 -0.974930

6 1.198487 3.431636 0.119137

1 2.146821 3.955689 0.177847

6 -0.023011 4.099630 0.197711

1 -0.027583 5.178941 0.320298

6 -1.238583 3.420497 0.127030

1 -2.191098 3.935977 0.192461

6 -3.612702 1.329731 -0.073252

1 -4.070219 2.302028 0.039668

6 -4.146037 0.093617 -0.203949

1 -5.175347 -0.235553 -0.226770

6 -3.268328 -2.248689 -0.459838

1 -2.393928 -2.669117 -0.957745

1 -4.163595 -2.444381 -1.053658

1 -3.380451 -2.702286 0.529544

6 0.004463 -2.925508 0.635117

8 0.015404 -4.253367 0.470183

8 0.003613 -2.318196 -0.488171

7 -0.011879 1.403350 -0.115613

1 0.019481 -4.452788 -0.492394

1 0.004933 -1.602517 2.086229

8 0.023750 -0.731809 2.553333

1 0.964378 -0.534749 2.624376

CBC-III-CO

2 2

28 0.000008 -0.803054 -0.008449

7 2.334731 0.990064 -0.016302

7 -2.334750 0.990031 -0.016162

7 -3.055062 -1.035179 -0.065760

7 3.055059 -1.035147 -0.065679

6 1.908509 -0.346637 -0.039310

6 1.289065 1.884967 0.003254

6 -1.289091 1.884952 0.003379

6 -1.908515 -0.346661 -0.039307

6 -4.160115 -0.188203 -0.056082

1 -5.167412 -0.580837 -0.077126

6 -3.706987 1.088877 -0.023374

1 -4.228388 2.034779 -0.010822

6 -3.168694 -2.488912 -0.085435

1 -2.574828 -2.895478 -0.906844

1 -4.215550 -2.751324 -0.242048

1 -2.835530 -2.901639 0.870293
6 -1.235880 3.257336 0.058913
1 -2.076955 3.942819 0.090145
6 1.235845 3.257354 0.058798
1 2.076916 3.942845 0.089956
6 3.706967 1.088918 -0.023540
1 4.228363 2.034825 -0.011081
6 4.160106 -0.188162 -0.056137
1 5.167405 -0.580792 -0.077150
6 3.168690 -2.488881 -0.085141
1 2.835201 -2.901483 0.870527
1 4.215596 -2.751317 -0.241380
1 2.575093 -2.895548 -0.906696
5 -0.000011 1.096330 -0.028341
7 -0.000018 3.836190 0.080745
1 -0.000021 4.855057 0.126485
6 0.000021 -2.656403 0.143381
8 0.000087 -3.790128 0.278716

CBC-III-CO_2^{2-}

0 2
28 0.000036 -0.646525 0.243301
7 -2.335374 1.066570 0.056753
7 2.335358 1.066653 0.056580
7 3.082330 -0.943102 0.168249
7 -3.082375 -0.943183 0.168162
6 -1.919056 -0.248561 0.178593
6 -1.274475 1.995944 0.048831
6 1.274440 1.996009 0.048722
6 1.919021 -0.248457 0.178500
6 4.177857 -0.103921 0.033398
1 5.187876 -0.489876 0.009155
6 3.706486 1.166251 -0.039680
1 4.219936 2.112224 -0.138449
6 3.190028 -2.391467 0.210411
1 2.315331 -2.800178 0.718635
1 4.097225 -2.669823 0.752689
1 3.239505 -2.798560 -0.805429
6 1.229602 3.336399 -0.189443
1 2.079472 3.995759 -0.351270
6 -1.229712 3.336339 -0.189330
1 -2.079626 3.995661 -0.351080
6 -3.706493 1.166194 -0.039596
1 -4.219924 2.112183 -0.138302
6 -4.177882 -0.103981 0.033264
1 -5.187901 -0.489929 0.008896
6 -3.190188 -2.391541 0.210259
1 -3.241093 -2.798468 -0.805578
1 -4.096695 -2.669899 0.753697
1 -2.314864 -2.800406 0.717279
5 0.000007 1.255909 0.254818
7 -0.000073 3.954196 -0.255495
1 -0.000106 4.953739 -0.417508
6 0.000128 -2.515503 -0.554330
8 0.000202 -2.894808 -1.710778
8 0.000076 -3.005124 0.588705

CBC-III-$COOH^-$

1 2
28 0.002901 -0.701123 -0.357898

7 2.355489 0.999581 -0.120147
7 -2.334064 1.024039 -0.146008
7 -3.056808 -0.976626 -0.446106
7 3.062543 -1.006849 -0.419967
6 1.927560 -0.290860 -0.331090
6 1.298493 1.926110 0.002788
6 -1.269353 1.940169 -0.012398
6 -1.916264 -0.269665 -0.357150
6 -4.164648 -0.156776 -0.295830
1 -5.170594 -0.550458 -0.344205
6 -3.708695 1.107872 -0.102563
1 -4.234065 2.038887 0.055859
6 -3.131800 -2.411944 -0.662091
1 -2.116972 -2.812262 -0.708733
1 -3.652315 -2.621691 -1.600508
1 -3.671640 -2.883049 0.163959
6 -1.209906 3.277195 0.257293
1 -2.056462 3.943321 0.402442
6 1.250239 3.263898 0.270850
1 2.102435 3.920880 0.424513
6 3.730644 1.072791 -0.077718
1 4.263248 1.999315 0.082846
6 4.176646 -0.195433 -0.271614
1 5.179530 -0.596815 -0.319783
6 3.124540 -2.438723 -0.664192
1 3.802272 -2.903410 0.056564
1 3.487402 -2.631820 -1.677702
1 2.122833 -2.858379 -0.545047
5 0.011654 1.228292 -0.172256
7 0.022864 3.871945 0.370831
1 0.027191 4.866686 0.567532
6 -0.035362 -2.042298 1.024533
8 -0.132282 -1.660697 2.307524
8 0.023621 -3.217794 0.706637
1 -0.135812 -2.471922 2.856279

CBC-III-H$^-$

1 2
28 -0.000003 -1.125222 0.000233
7 2.350822 0.692321 0.000118
7 -2.350820 0.692320 0.000110
7 -3.111471 -1.315768 -0.000096
7 3.111468 -1.315768 -0.000088
6 1.956968 -0.624788 0.000284
6 1.277392 1.608759 0.000104
6 -1.277391 1.608757 0.000104
6 -1.956968 -0.624789 0.000280
6 -4.200718 -0.460967 -0.000433
1 -5.213933 -0.838338 -0.000715
6 -3.720490 0.809728 -0.000398
1 -4.227075 1.764154 -0.000596
6 -3.247440 -2.764007 -0.000036
1 -2.249618 -3.206788 0.000051
1 -3.793875 -3.080884 -0.892373
1 -3.794067 -3.080818 0.892202
6 -1.227531 2.973284 0.000051
1 -2.078868 3.649217 -0.000013
6 1.227532 2.973285 0.000056
1 2.078869 3.649219 -0.000004
6 3.720492 0.809726 -0.000330

1 4.227078 1.764152 -0.000472

6 4.200718 -0.460969 -0.000520

1 5.213932 -0.838343 -0.000874

6 3.247443 -2.764007 -0.000017

1 3.794108 -3.080807 0.892202

1 3.793844 -3.080886 -0.892374

1 2.249624 -3.206793 0.000115

1 0.000017 -2.756553 -0.000323

5 0.000001 0.875690 0.000253

7 0.000000 3.585175 0.000031

1 -0.000001 4.599213 -0.000009

CBC-III-H-CO_2

1 2

28 0.004676 -0.640503 -0.487395

7 2.332338 1.152740 -0.060085

7 -2.369542 1.091696 -0.065850

7 -3.083591 -0.906097 -0.405224

7 3.102302 -0.822283 -0.410108

6 1.947682 -0.138287 -0.326955

6 1.247021 2.034994 0.137623

6 -1.308336 2.002511 0.132918

6 -1.949220 -0.188778 -0.328896

6 -4.192007 -0.100106 -0.201825

1 -5.195289 -0.502368 -0.226847

6 -3.741575 1.164404 0.008744

1 -4.270324 2.086724 0.202744

6 -3.157722 -2.347427 -0.585238

1 -2.213472 -2.694576 -1.011827

1 -3.982671 -2.586915 -1.260121

1 -3.323382 -2.835550 0.380227

6 -1.275777 3.351643 0.341475

1 -2.135465 4.011396 0.425303

6 1.178962 3.382977 0.346363

1 2.021079 4.064735 0.433121

6 3.701920 1.264455 0.010564

1 4.205169 2.200561 0.206292

6 4.187573 0.014178 -0.206285

1 5.201935 -0.358851 -0.235539

6 3.218651 -2.260077 -0.598092

1 3.366017 -2.752138 0.368393

1 4.070700 -2.472003 -1.247948

1 2.298170 -2.628578 -1.057051

6 0.062115 -3.060975 1.253103

8 -0.002765 -1.942292 1.594770

8 0.125995 -4.183472 0.964367

1 0.023658 -2.108498 -1.218884

5 -0.021162 1.286563 0.060466

7 -0.056273 3.969187 0.454436

1 -0.069425 4.969675 0.620586

CBC-III-$HCOO^-$

1 2

28 -0.000001 -0.729220 -0.211091

7 -2.356828 1.055958 -0.069631

7 2.356774 1.056032 -0.069622

7 3.110767 -0.945467 -0.241320

7 -3.110755 -0.945571 -0.241271

6 -1.962525 -0.249548 -0.211669

6 -1.279834 1.961802 0.019063

6 1.279752 1.961841 0.019088

6 1.962513 -0.249479 -0.211752

6 4.203943 -0.102195 -0.118344

1 5.215585 -0.483774 -0.125201

6 3.728067 1.165213 -0.009944

1 4.236774 2.112377 0.098094

6 3.213697 -2.394676 -0.328325

1 3.390942 -2.815929 0.666328

1 4.044790 -2.657607 -0.986642

1 2.279280 -2.791205 -0.728768

6 1.226332 3.322036 0.135486

1 2.078952 3.993758 0.190186

6 -1.226459 3.321999 0.135469

1 -2.079101 3.993693 0.190158

6 -3.728128 1.165105 -0.010044

1 -4.236867 2.112260 0.097915

6 -4.203963 -0.102322 -0.118423

1 -5.215594 -0.483929 -0.125326

6 -3.213621 -2.394794 -0.328116

1 -2.279239 -2.791318 -0.728645

1 -4.044792 -2.657832 -0.986293

1 -3.390704 -2.815954 0.666605

6 0.000107 -2.894320 0.903343

8 0.000160 -1.842037 1.594536

8 0.000036 -2.865960 -0.358080

1 0.000196 -3.871193 1.423590

5 -0.000029 1.234536 -0.032135

7 -0.000073 3.930659 0.191654

1 -0.000090 4.940824 0.283902

CBC-III

0 2

28 0.000000 -0.991281 -0.199999

7 -2.314329 0.647676 -0.061210

7 2.314324 0.647678 -0.061205

7 3.053161 -1.367132 0.107702

7 -3.053155 -1.367138 0.107699

6 -1.891736 -0.673650 -0.039476

6 -1.268123 1.584150 -0.223580

6 1.268117 1.584149 -0.223580

6 1.891739 -0.673651 -0.039478

6 4.150847 -0.521319 0.178344

1 5.157423 -0.901187 0.291044

6 3.684304 0.749134 0.080862

1 4.202882 1.697818 0.092279

6 3.131615 -2.811189 0.176720

1 2.129548 -3.201312 0.379886

1 3.806336 -3.112381 0.983695

1 3.494424 -3.231128 -0.767346

6 1.226046 2.895577 0.134529

1 2.072317 3.512292 0.432192

6 -1.226054 2.895578 0.134526

1 -2.072325 3.512293 0.432187

6 -3.684315 0.749123 0.080802

1 -4.202903 1.697802 0.092169

6 -4.150839 -0.521328 0.178407

1 -5.157408 -0.901198 0.291159

6 -3.131602 -2.811196 0.176713

1 -3.494450 -3.231135 -0.767338

1 -3.806286 -3.112392 0.983717

1 -2.129524 -3.201314 0.379835

5 -0.000003 0.871756 -0.643059

7 -0.000003 3.535694 0.177012

1 -0.000003 4.519207 0.413068

C(B)NC-II-CO

1 1

28 0.000024 -0.672540 0.004480

7 2.230386 0.919625 -0.002995

7 -2.230287 0.919751 -0.003443

7 -3.065240 -1.057863 -0.022954

7 3.065197 -1.058031 -0.023304

6 1.899168 -0.398830 -0.006369

6 1.174614 1.865043 0.005149

6 -1.174480 1.865125 0.004848

6 -1.899143 -0.398734 -0.006340

6 -4.123191 -0.161891 -0.030089

1 -5.149077 -0.501407 -0.044063

6 -3.598647 1.088610 -0.017792

1 -4.069251 2.061164 -0.019568

6 -3.223758 -2.506223 -0.032417

1 -2.742603 -2.930375 -0.917265

1 -4.289283 -2.736602 -0.066421

1 -2.799285 -2.936174 0.878445

6 -1.291145 3.223015 0.021165

1 -2.295847 3.642842 0.029042

6 1.291348 3.222928 0.021527

1 2.296071 3.642695 0.029687

6 3.598762 1.088390 -0.017440

1 4.069434 2.060912 -0.018955

6 4.123230 -0.162149 -0.029923

1 5.149089 -0.501746 -0.043875

6 3.223464 -2.506408 -0.033088

1 2.800011 -2.936341 0.878255

1 4.288891 -2.737015 -0.068534

1 2.741009 -2.930365 -0.917326

7 0.000041 1.189670 -0.006141

5 0.000128 4.025715 0.030463

1 0.000167 5.226039 0.045935

6 -0.000160 -2.451646 0.052557

8 -0.000210 -3.589568 0.097254

C(B)NC-II-CO_2^{2-}

-1 1

28 0.000000 -0.621777 -0.011657

7 -2.220681 1.040481 0.007103

7 2.220682 1.040479 0.007094

7 3.106537 -0.908530 0.111299

7 -3.106537 -0.908528 0.111289

6 -1.902936 -0.302009 0.046224

6 -1.165762 2.007132 -0.024281

6 1.165764 2.007131 -0.024289

6 1.902937 -0.302012 0.046217

6 4.147343 0.010378 0.105354

1 5.182873 -0.297798 0.152279

6 3.587256 1.242287 0.043106

1 4.036766 2.225215 0.028420

6 3.293229 -2.349207 0.155931

1 2.384565 -2.805297 0.558543

1 4.144247 -2.584070 0.800972

1 3.485314 -2.742843 -0.847680
6 1.295639 3.376273 -0.047188
1 2.299528 3.802225 -0.048780
6 -1.295636 3.376275 -0.047188
1 -2.299525 3.802227 -0.048782
6 -3.587257 1.242288 0.043040
1 -4.036768 2.225215 0.028296
6 -4.147340 0.010385 0.105456
1 -5.182867 -0.297788 0.152458
6 -3.293227 -2.349206 0.155882
1 -3.485345 -2.742818 -0.847732
1 -4.144221 -2.584087 0.800948
1 -2.384546 -2.805303 0.558447
7 0.000001 1.358169 -0.017783
5 0.000002 4.169123 -0.062939
1 0.000003 5.376522 -0.083056
6 -0.000006 -2.496911 -0.184570
8 -0.000005 -2.820329 -1.388857
8 -0.000004 -3.204494 0.846553

C(B)NC-II-COOH$^-$

0 1
28 -0.000004 -0.544191 -0.043224
7 2.223781 1.065263 -0.010273
7 -2.223769 1.065282 -0.010273
7 -3.084012 -0.898161 -0.034111
7 3.084005 -0.898188 -0.034112
6 1.897467 -0.266145 -0.029954
6 1.169056 2.023364 -0.003241
6 -1.169031 2.023371 -0.003238
6 -1.897469 -0.266128 -0.029955
6 -4.133908 0.009093 -0.009317
1 -5.164798 -0.316036 -0.009297
6 -3.591404 1.250664 0.003476
1 -4.051651 2.228334 0.013941
6 -3.266217 -2.341880 -0.014055
1 -2.480158 -2.814504 -0.605694
1 -4.238376 -2.580271 -0.450717
1 -3.230681 -2.716129 1.013304
6 -1.293308 3.386883 0.038769
1 -2.297624 3.808970 0.063686
6 1.293344 3.386874 0.038768
1 2.297662 3.808955 0.063686
6 3.591418 1.250634 0.003482
1 4.051674 2.228299 0.013949
6 4.133909 0.009057 -0.009312
1 5.164795 -0.316082 -0.009290
6 3.266200 -2.341909 -0.014063
1 3.230650 -2.716163 1.013294
1 4.238363 -2.580302 -0.450715
1 2.480145 -2.814524 -0.605714
7 0.000011 1.362322 -0.035244
5 0.000021 4.183921 0.058022
1 0.000025 5.387707 0.095810
6 -0.000014 -2.395834 -0.059625
8 -0.000021 -2.953148 1.181420
8 -0.000023 -3.123482 -1.040833
1 -0.000037 -3.921360 1.046917

C(B)NC-II-H-CO_2

0 1

28 -0.008169 -0.408289 -0.432290

7 2.254790 1.086796 -0.067155

7 -2.189834 1.197162 -0.044999

7 -3.077638 -0.721046 -0.411428

7 3.038387 -0.879459 -0.418154

6 1.880106 -0.202415 -0.350233

6 1.227764 2.055685 0.128540

6 -1.114165 2.113148 0.143107

6 -1.884021 -0.109034 -0.334127

6 -4.114148 0.172215 -0.175509

1 -5.148740 -0.140489 -0.195724

6 -3.554119 1.385150 0.053900

1 -4.001538 2.344556 0.271700

6 -3.268279 -2.145087 -0.629000

1 -4.125075 -2.302636 -1.288643

1 -3.447164 -2.652837 0.324361

1 -2.368014 -2.552455 -1.093234

6 -1.203523 3.453072 0.414080

1 -2.197273 3.892801 0.497985

6 1.385313 3.390109 0.395915

1 2.399978 3.781677 0.466020

6 3.627023 1.200759 0.036368

1 4.124935 2.135845 0.250873

6 4.121339 -0.042123 -0.183801

1 5.137772 -0.409976 -0.198359

6 3.149178 -2.314212 -0.618717

1 3.341403 -2.814647 0.335694

1 3.968676 -2.526719 -1.309780

1 2.210251 -2.681119 -1.038478

6 -0.103706 -3.524246 1.148619

8 0.039801 -2.740046 1.998916

8 -0.248647 -4.340057 0.329198

1 -0.045151 -1.829201 -0.843771

7 0.040079 1.437044 0.012693

5 0.111004 4.200976 0.565322

1 0.141351 5.381638 0.802380

C(B)NC-II-H$^-$

0 1

28 0.000006 -0.952806 -0.000162

7 -2.223036 0.644409 0.000013

7 2.223036 0.644415 0.000016

7 3.069154 -1.326219 0.000049

7 -3.069159 -1.326221 0.000058

6 -1.887216 -0.686756 0.000006

6 -1.170762 1.605207 -0.000062

6 1.170758 1.605211 -0.000054

6 1.887214 -0.686748 -0.000001

6 4.126327 -0.425742 0.000049

1 5.154806 -0.758728 0.000214

6 3.592371 0.819641 -0.000077

1 4.059920 1.794066 -0.000030

6 3.245347 -2.768066 0.000173

1 2.259759 -3.237153 -0.001456

1 3.796839 -3.076165 0.892949

1 3.799664 -3.075875 -0.890942

6 1.294289 2.969500 0.000137

1 2.298790 3.392091 0.000465

6 -1.294295 2.969497 0.000141

1 -2.298797 3.392086 0.000475

6 -3.592370 0.819638 -0.000013

1 -4.059917 1.794064 0.000086

6 -4.126330 -0.425742 -0.000060

1 -5.154809 -0.758727 0.000021

6 -3.245350 -2.768068 0.000225

1 -3.799671 -3.075897 -0.890879

1 -3.796838 -3.076147 0.893012

1 -2.259762 -3.237155 -0.001398

7 -0.000001 0.945295 -0.000299

5 -0.000004 3.765794 0.000115

1 -0.000007 4.970384 -0.000011

1 0.000038 -2.434435 -0.000200

C(B)NC-II-HCOO$^-$

0 1

28 0.000021 -0.544970 -0.213997

7 -2.232605 1.044234 -0.030090

7 2.232966 1.043862 -0.030958

7 3.074524 -0.916998 -0.230283

7 -3.074672 -0.916293 -0.230462

6 -1.900838 -0.271176 -0.176751

6 -1.172362 1.983809 0.055449

6 1.172927 1.983621 0.054902

6 1.900875 -0.271499 -0.177336

6 4.133249 -0.025836 -0.111633

1 5.160843 -0.360846 -0.132743

6 3.603357 1.215498 0.011584

1 4.072446 2.183088 0.118466

6 3.229541 -2.359185 -0.349303

1 3.350966 -2.809449 0.640955

1 4.112458 -2.575784 -0.955007

1 2.339114 -2.767037 -0.829896

6 1.290059 3.339171 0.194978

1 2.295830 3.755256 0.245072

6 -1.289219 3.339371 0.195660

1 -2.294901 3.755609 0.246291

6 -3.602962 1.216282 0.011865

1 -4.071803 2.183967 0.118961

6 -4.133176 -0.024828 -0.112193

1 -5.160860 -0.359532 -0.133802

6 -3.230123 -2.358374 -0.350168

1 -2.339815 -2.766300 -0.830914

1 -4.113120 -2.574385 -0.955962

1 -3.351745 -2.809088 0.639867

6 -0.000786 -3.085746 0.614567

8 -0.000199 -2.404881 -0.477860

5 0.000502 4.136586 0.272363

1 0.000625 5.333715 0.392788

1 -0.001311 -4.184161 0.422850

8 -0.000800 -2.659386 1.764134

7 0.000206 1.316433 -0.023454

C(B)NC-II

-1 1

28 0.000000 -1.030024 0.066450

7 -2.203271 0.626105 -0.097070

7 2.203270 0.626105 -0.097068

7 3.094889 -1.324230 0.008790

7 -3.094889 -1.324230 0.008792

6 -1.874098 -0.720689 0.052033
6 -1.161576 1.606853 -0.094276
6 1.161575 1.606853 -0.094272
6 1.874098 -0.720690 0.052033
6 4.130408 -0.411879 -0.138469
1 5.165473 -0.721977 -0.190637
6 3.567569 0.818406 -0.197193
1 4.013181 1.796397 -0.317025
6 3.300250 -2.753233 0.124627
1 2.338696 -3.212471 0.375033
1 4.027719 -2.969648 0.913812
1 3.663336 -3.172129 -0.819742
6 1.294280 2.954157 0.170615
1 2.296070 3.348937 0.350799
6 -1.294280 2.954156 0.170614
1 -2.296071 3.348936 0.350797
6 -3.567570 0.818407 -0.197174
1 -4.013184 1.796399 -0.316990
6 -4.130405 -0.411882 -0.138498
1 -5.165469 -0.721982 -0.190689
6 -3.300251 -2.753232 0.124643
1 -3.663340 -3.172134 -0.819721
1 -4.027717 -2.969640 0.913832
1 -2.338696 -3.212469 0.375049
7 0.000000 0.987836 -0.312103
5 0.000000 3.741989 0.281587
1 -0.000001 4.928047 0.519447

C(B)NC-III-CO_2^{2-}

0 2
28 -0.000325 -0.537687 0.313509
7 -2.215234 1.107962 0.048944
7 2.242192 1.069176 0.042948
7 3.139409 -0.863715 0.260564
7 -3.146933 -0.807767 0.272365
6 -1.932179 -0.226560 0.235817
6 -1.146171 2.058612 -0.062092
6 1.189598 2.038388 -0.064665
6 1.935678 -0.260233 0.228048
6 4.175140 0.044591 0.096024
1 5.211781 -0.262642 0.095549
6 3.607288 1.267389 -0.038598
1 4.052486 2.242561 -0.176579
6 3.321892 -2.298997 0.386257
1 2.469771 -2.717392 0.926678
1 4.237994 -2.504015 0.945748
1 3.391503 -2.766424 -0.601669
6 1.330120 3.390996 -0.260533
1 2.336174 3.804660 -0.333392
6 -1.263668 3.413437 -0.257929
1 -2.262567 3.844478 -0.328710
6 -3.576518 1.330833 -0.030484
1 -4.004002 2.313678 -0.169784
6 -4.166308 0.118944 0.107912
1 -5.208326 -0.169562 0.110116
6 -3.357879 -2.238584 0.402811
1 -3.466452 -2.703131 -0.582951
1 -4.261224 -2.424505 0.989118
1 -2.499276 -2.675844 0.917769
7 0.016294 1.411822 0.038790

5 0.039931 4.187723 -0.369081

1 0.050044 5.381385 -0.542728

6 -0.053439 -3.282989 -0.783146

8 -0.112058 -2.982260 -1.907070

8 0.003324 -3.618229 0.334092

C(B)NC-III-H$^-$

1 2

28 0.000000 -0.933341 -0.000052

7 -2.219523 0.649732 -0.000017

7 2.219523 0.649732 -0.000024

7 3.053589 -1.341925 0.000041

7 -3.053589 -1.341925 0.000062

6 -1.881992 -0.688822 -0.000046

6 -1.173544 1.616769 -0.000047

6 1.173544 1.616769 -0.000047

6 1.881992 -0.688822 -0.000050

6 4.103690 -0.453260 0.000200

1 5.132046 -0.787068 0.000328

6 3.577909 0.807058 0.000061

1 4.059619 1.774821 0.000080

6 3.210622 -2.789816 -0.000027

1 2.218750 -3.244616 0.000009

1 3.760310 -3.096493 0.893133

1 3.760216 -3.096433 -0.893266

6 1.296979 2.980861 -0.000060

1 2.299964 3.404886 -0.000061

6 -1.296979 2.980861 -0.000045

1 -2.299964 3.404886 -0.000033

6 -3.577909 0.807058 0.000138

1 -4.059619 1.774821 0.000216

6 -4.103690 -0.453260 0.000086

1 -5.132046 -0.787068 0.000128

6 -3.210622 -2.789816 0.000036

1 -3.760166 -3.096458 -0.893225

1 -3.760360 -3.096468 0.893174

1 -2.218750 -3.244616 0.000140

1 0.000000 -2.389429 -0.000067

5 0.000000 3.778318 -0.000060

1 0.000000 4.978544 -0.000070

7 0.000000 0.965697 -0.000052

C(B)NC-I

0 2

28 -0.000001 -1.034784 0.000033

7 -2.229571 0.616536 0.000419

7 2.229571 0.616535 0.000410

7 3.153202 -1.315773 -0.000184

7 -3.153202 -1.315773 -0.000177

6 -1.939108 -0.730743 0.000272

6 -1.167673 1.581577 0.000435

6 1.167673 1.581577 0.000435

6 1.939108 -0.730743 0.000269

6 4.177706 -0.379706 -0.000246

1 5.218950 -0.671373 -0.000379

6 3.592898 0.841914 -0.000016

1 4.025300 1.832457 -0.000091

6 3.373601 -2.750157 -0.000311

1 2.402339 -3.249736 -0.000834

1 3.933819 -3.046605 0.891422

1 3.934619 -3.046289 -0.891641
6 1.296677 2.949644 -0.000342
1 2.298963 3.378504 -0.000863
6 -1.296677 2.949644 -0.000323
1 -2.298962 3.378504 -0.000826
6 -3.592899 0.841914 0.000098
1 -4.025300 1.832457 0.000115
6 -4.177706 -0.379706 -0.000395
1 -5.218950 -0.671373 -0.000649
6 -3.373600 -2.750157 -0.000270
1 -3.934580 -3.046308 -0.891618
1 -3.933856 -3.046587 0.891446
1 -2.402338 -3.249736 -0.000743
7 0.000000 0.936972 0.001083
5 0.000000 3.742279 -0.000672
1 0.000000 4.948829 -0.001388

TS-CBC-III-H-CO_2

1 2
28 0.000000 -0.676340 -0.343587
7 2.351912 1.111208 -0.062694
7 -2.351909 1.111212 -0.062693
7 -3.102456 -0.876161 -0.377119
7 3.102456 -0.876166 -0.377117
6 1.953638 -0.184411 -0.280442
6 1.278805 2.013797 0.101212
6 -1.278801 2.013800 0.101213
6 -1.953637 -0.184407 -0.280445
6 -4.196797 -0.040868 -0.223634
1 -5.208141 -0.420086 -0.271799
6 -3.723130 1.217294 -0.027830
1 -4.235251 2.156031 0.127862
6 -3.209645 -2.316995 -0.550374
1 -2.301156 -2.683625 -1.032731
1 -4.076788 -2.539258 -1.176032
1 -3.328199 -2.804422 0.422478
6 -1.227536 3.367045 0.279419
1 -2.078606 4.038942 0.353901
6 1.227543 3.367043 0.279418
1 2.078614 4.038939 0.353899
6 3.723133 1.217289 -0.027834
1 4.235255 2.156025 0.127853
6 4.196798 -0.040875 -0.223637
1 5.208142 -0.420094 -0.271802
6 3.209643 -2.317002 -0.550364
1 3.328174 -2.804425 0.422492
1 4.076799 -2.539270 -1.176002
1 2.301163 -2.683631 -1.032739
6 -0.000005 -2.925194 0.968298
8 -0.000006 -1.899842 1.582344
8 -0.000006 -4.087369 0.797959
1 -0.000001 -2.275225 -0.772906
5 0.000001 1.285958 0.031944
7 0.000004 3.971397 0.371378
1 0.000005 4.975993 0.511541

TS-C(B)NC-II-H-CO_2

0 1
28 0.000125 -0.488409 -0.061367
7 2.230478 1.098465 -0.029082

7 -2.231963 1.095999 -0.029387
7 -3.062738 -0.879504 -0.110111
7 3.063489 -0.876086 -0.109992
6 1.894155 -0.220987 -0.083370
6 1.174045 2.041269 0.007385
6 -1.176572 2.039969 0.007215
6 -1.894154 -0.223070 -0.083655
6 -4.125445 0.014268 -0.067440
1 -5.151049 -0.326731 -0.081453
6 -3.603430 1.263665 -0.018452
1 -4.076801 2.234284 0.016555
6 -3.219030 -2.326448 -0.123035
1 -4.175405 -2.572829 -0.588715
1 -3.199714 -2.719716 0.897264
1 -2.412141 -2.778221 -0.703593
6 -1.291453 3.401106 0.052304
1 -2.297641 3.818664 0.063114
6 1.287416 3.402532 0.052483
1 2.293131 3.821227 0.063442
6 3.601749 1.267686 -0.018262
1 4.074018 2.238840 0.016747
6 4.125178 0.018887 -0.067353
1 5.151166 -0.320948 -0.081461
6 3.221443 -2.322861 -0.123124
1 3.202487 -2.716283 0.897131
1 4.178157 -2.568052 -0.588736
1 2.415110 -2.775526 -0.703770
6 0.002170 -2.885739 0.085765
8 0.000248 -2.405188 1.237485
8 0.005371 -4.029171 -0.350126
1 0.000634 -2.084874 -0.807447
7 -0.000892 1.369939 -0.010581
5 -0.002464 4.202555 0.080337
1 -0.003128 5.404348 0.119949

CBC-III-H_2O-$OCHO^-$

1 2
28 -0.025048 -0.528113 -0.150889
7 -2.273938 1.396041 -0.090220
7 2.436079 1.116412 -0.100893
7 3.082428 -0.917544 -0.319792
7 -3.154803 -0.544674 -0.331733
6 -1.963080 0.069469 -0.247493
6 -1.143715 2.231412 0.017507
6 1.411617 2.079104 0.008420
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6 4.219878 -0.130522 -0.240691
1 5.210208 -0.561162 -0.294555
6 3.812237 1.158086 -0.103441
1 4.371439 2.078559 -0.015834
6 3.105677 -2.369540 -0.421232
1 3.196771 -2.814159 0.574966
1 3.960258 -2.670414 -1.031291
1 2.177746 -2.707427 -0.884673
6 1.439532 3.439967 0.119091
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1 -4.264141 -2.165743 -1.030763
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8 -0.371121 -4.512220 0.463920
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1 5.150124 -0.166310 -0.312133
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1 4.032563 2.359787 -0.013201
6 3.249077 -2.188430 -0.510787
1 3.360817 -2.653047 0.474128
1 4.145681 -2.380415 -1.104385
1 2.376785 -2.608911 -1.012722
6 1.242325 3.479539 0.116194
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6 -1.335891 3.454683 0.140713
1 -2.345111 3.861080 0.199870
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1 -4.107539 2.281018 0.061808
6 -4.154300 0.074356 -0.189962
1 -5.179722 -0.266906 -0.216181
6 -3.241632 -2.251019 -0.449127
1 -2.370585 -2.654012 -0.967295
1 -4.145335 -2.461924 -1.025340
1 -3.324794 -2.716628 0.538026
6 0.026694 -2.920670 0.593836
8 0.003889 -4.247407 0.389363
8 -0.005964 -2.282254 -0.508330
7 -0.029553 1.445015 -0.097623
1 -0.034279 -4.411703 -0.578839
1 0.165853 -1.689926 2.123200
8 0.243814 -0.893658 2.703015
1 1.105956 -0.534416 2.468048
5 -0.053832 4.264074 0.211732
1 -0.063950 5.460314 0.339229