Charge Transfer Reactions between Gas-Phase Hydrated Electrons, Molecular Oxygen and Carbon Dioxide at Temperatures of 80 - 300 K

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Electronic supplementary information (ESI)

Conversion of ΔE_{raw} to ΔH_{298K}

Reaction (3)

Temperatures in the experiment:

$(H_2O)_n^-$	+ CO_2	→	$CO_2^-(H_2O)_m$	+ (n-m) H_2O
90 - 120 K	298 K		90-120 K	120-160 K

The internal temperature of water clusters is a result of radiative heating and evaporative cooling. We assume here a value of 90 – 120 K, which corresponds to the region where the solid-to-liquid phase transition occurs in hydrated electrons (Hock *et al.*, *Phys. Rev. Lett.*, 2009, **103**, 73401). The neutral reactant is at room temperature, equilibrated in collisions with the surfaces in the UHV region of the mass spectrometer. The neutral products, including the evaporating H_2O molecules, will have an internal energy distribution that corresponds to the internal temperature of the cluster after the reaction. The heat of the reaction is heating the cluster with $\Delta E_{raw} = 107$ kJ mol^{-1}. Setting n = 50, there are about 6n = 300 low-lying vibrational degrees of freedom which correspond to the translational and rotational degrees of freedom of the free water molecules. If we assume that these are thermally populated, we have 0.36 kJ mol^{-1} per degree of freedom. A fully populated vibrational degree of freedom contains RT internal energy, therefore the 0.36 kJ mol^{-1} per degree of freedom correspond to a temperature increase of 43 K. Of course, the cluster immediately responds with evaporative cooling, therefore we do not know the exact temperature at which each neutral molecule evaporates. In addition, instead of increasing the temperature, the cluster may convert the additional energy into latent heat by breaking hydrogen bonds. Since a detailed modeling of all these aspects goes beyond the scope of the present work, we give the conservative range above.

From nanocalorimetry, we obtain ΔE_{raw} at these conditions:

$\Delta E_{raw}(3) = -\Delta N_{vap}\, \Delta E_{vap} = -107 \pm 39$ kJ mol^{-1}

Corrections for ΔH_{298K}:

The difference in heat capacity of a hydrated electron compared to hydrated CO_2^- is unknown. However, the three translational and three rotational degrees of freedom of free, bent CO_2^- are converted to six low-lying vibrational degrees of freedom of the CO_2^- ion oscillating in the cluster provide an upper limit. If these low-lying modes are thermally populated, we have a contribution to the heat capacity of 6*R*. Since the heat of the reaction has to provide the energy to populate these modes, this effect reduces the exothermicity, therefore the correction has a positive sign. Since the correction lies somewhere between 0 and 6 *RT*, we suggest:

$\Delta(\Delta H)_C = 3 \pm 3\ [R(298\ \text{K} - 105\ \text{K})] = 4.8 \pm 4.8$ kJ mol^{-1}

The neutral reactant has room temperature. Considering enthalpy at standard conditions, we have to consider the volume work term pV = RT, which must be subtracted from ΔE_{raw}.

$pV = RT = 2.5$ kJ mol^{-1}

In summary, we obtain with Gaussian error propagation:

$\Delta H_{298K}(3) = \Delta E_{raw} + \Delta(\Delta H)_C$ -pV $= -107 + 4.8 - 2.5 \pm \text{sqrt}(39^2 + 4.0^2)$ kJ mol^{-1}

$= -105 \pm 39$ kJ mol^{-1}

Reaction (4)

$(H_2O)_n^-$	$+ O_2$	→	$O_2^-(H_2O)_m$	$+ (n\text{-}m)\ H_2O$
90 - 120 K	298 K		90-120 K	120-230 K

With similar arguments as above, the heat of the reaction is heating the cluster with ΔE_{raw} = 277 kJ mol^{-1}. Again for 300 low-lying internal degrees of freedom, which we assume to be thermally populated, we have 0.92 kJ mol^{-1} per degree of freedom, corresponding to a temperature increase of 111 K.

From nanocalorimetry, we obtain $\boldsymbol{\Delta E_{raw}}$ at these conditions:

$$\Delta E_{raw} = -\Delta N_{vap}\ \Delta E_{vap} = -277 \pm 28 \text{ kJ mol}^{-1}$$

Corrections for ΔH_{298K}:

The difference in heat capacity of a hydrated electron compared to hydrated O_2^- is unknown. However, the three translational and two rotational degrees of freedom of free O_2 are converted to five low-lying vibrational degrees of freedom of the O_2^- ion oscillating in the cluster provide an upper limit. If these low-lying modes are thermally populated, we have a contribution to the heat capacity of 5*R*. Since the heat of the reaction has to provide the energy to populate these modes, this effect reduces the exothermicity, therefore the correction has a positive sign. Since the correction lies somewhere between 0 and 5 *RT*, we suggest:

$$\Delta(\Delta H)_C = 2.5 \pm 2.5\ [R(298 \text{ K} - 105 \text{ K})] = 4.0 \pm 4.0 \text{ kJ mol}^{-1}$$

The neutral reactant has room temperature. Considering enthalpy at standard conditions, we have to consider the volume work term pV = RT, which must be subtracted from ΔE_{raw}.

$pV = RT = 2.5$ kJ mol^{-1}

In summary, we obtain with Gaussian error propagation:

$$\Delta H_{298K}(4) = \Delta E_{raw} + \Delta(\Delta H)_C \text{ -pV} = -277 + 4.0 - 2.5 \pm \text{sqrt}(28^2 + 4.0^2) \text{ kJ mol}^{-1}$$
$$= -276 \pm 28 \text{ kJ mol}^{-1}$$

Reaction (5)

$CO_2^-(H_2O)_n^-$	+	O_2	→	$O_2^-(H_2O)_m$	+	$CO_2 + (n\text{-}m)\ H_2O$
90 - 120 K		298 K		90-120 K		120-180 K

With similar arguments as above, the heat of the reaction is heating the cluster with ΔE_{raw} = 147 kJ mol^{-1}. Again for 300 low-lying internal degrees of freedom, which we assume to be thermally populated, we have 0.5 kJ mol^{-1} per degree of freedom, corresponding to a temperature increase of 60 K.

From nanocalorimetry, we obtain $\boldsymbol{\Delta E_{raw}}$ at these conditions:

$$\Delta E_{raw} = -\Delta N_{vap}\ \Delta E_{vap} = -147 \pm 29 \text{ kJ mol}^{-1}$$

Corrections for ΔH_{298K}:

The difference in heat capacity of a hydrated CO_2^- compared to hydrated O_2^- is unknown. With the arguments above, we have a contribution of 6*R* for CO_2^- and 5*R* for O_2^-. I.e. on the

product side, the heat capacity is on the order of 1R lower. This results in a correction with a negative sign:

$\Delta(\Delta H)_C = -1 \pm 0.5\ [R(298\ \mathrm{K} - 105\ \mathrm{K})] = -1.6 \pm 0.8\ \mathrm{kJ\ mol^{-1}}$

Similar arguments apply to the neutral reactant and product. For $\Delta H_{298\mathrm{K}}$, the CO_2 must be heated to 298 K. The heat capacity of a rigid linear rotor without thermally populated vibrational levels is 5/2R. The correction therefore amounts to:

$\Delta(\Delta H)_{CO2} = 5/2R(298\ \mathrm{K} - (165 \pm 45\mathrm{K})] = 2.8 \pm 0.9\ \mathrm{kJ\ mol^{-1}}$

The $pV = RT$ contribution is the same on the left and right hand side.

In summary, we obtain with Gaussian error propagation:

$\Delta H_{298\mathrm{K}}(5) = \Delta E_{\mathrm{raw}} + \Delta(\Delta H)_C + \Delta(\Delta H)_{CO2} = -147-1.6+2.8 \pm \mathrm{sqrt}(29^2+0.8^2+0.9^2)\ \mathrm{kJ\ mol^{-1}}$

$= -146 \pm 29\ \mathrm{kJ\ mol^{-1}}$

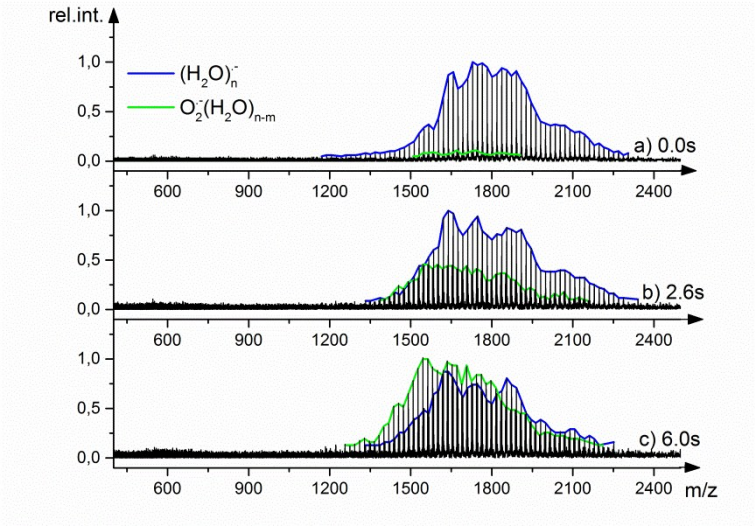

Figure S1: Mass spectra of reaction (4), $(H_2O)_n^-$ with O_2 at T = 136 K and p = $5.2 \cdot 10^{-9}$ mbar. a) At the beginning of the reaction the reactant clusters are the dominant species. b) After 2.6s the product clusters distribution is increased to half the quantity of the reactant clusters. c) At 6s the charge transfer is still not completed and more than half of the reactants are converted to $O_2^{\bullet -}(H_2O)_{n-m}$.

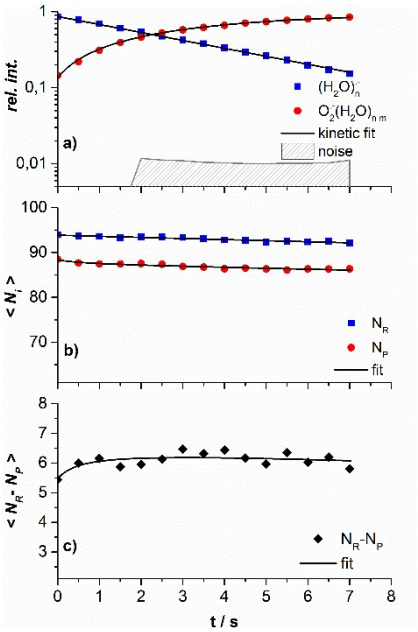

Figure S2: a) kinetics and (b and c) nanocalorimetric fits of the reaction of $(H_2O)_n^-$ with O_2 at T = 140 K and p = $8.0 \cdot 10^{-9}$ mbar. Blue filled square, $(H_2O)_n^-$; red filled circle, $O_2^{\bullet-}(H_2O)_{n-m}$; filled diamond, difference in the cluster size.

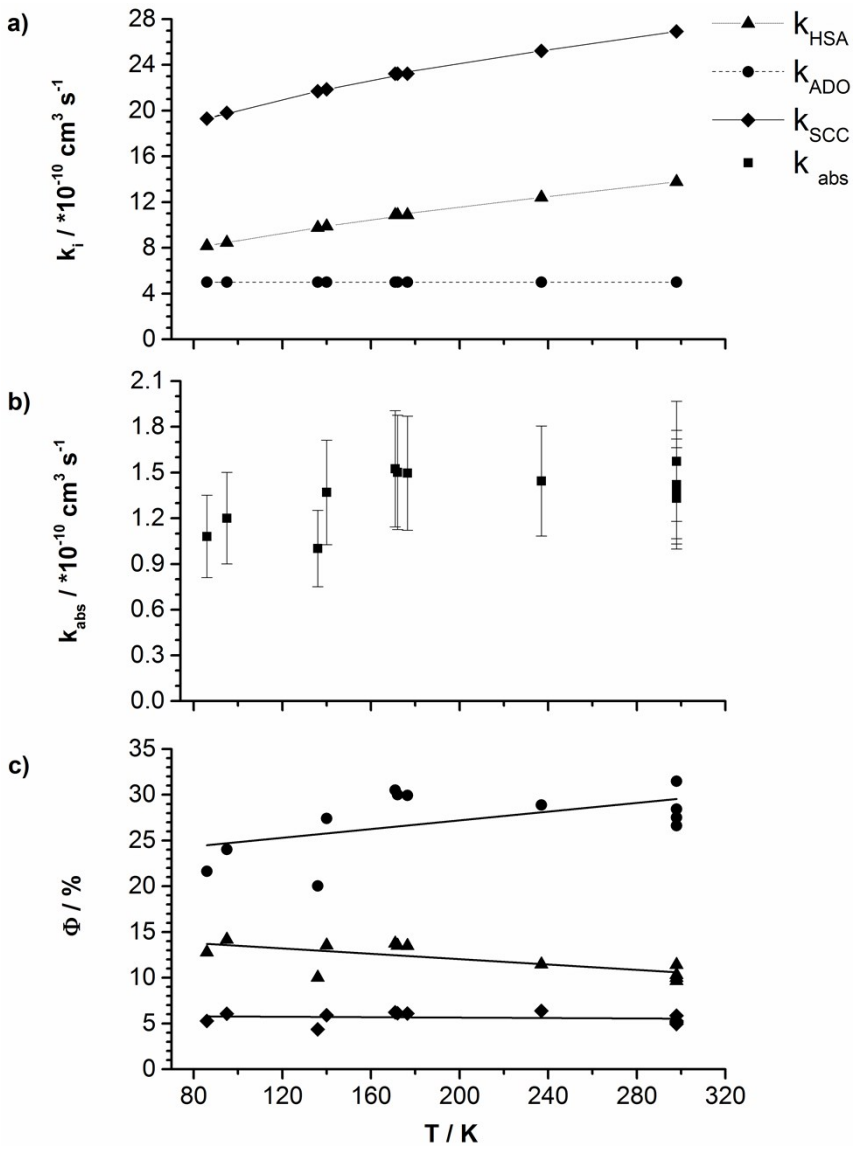

Figure S3: Kinetic analysis of reaction (4). (a) Calculated collision rates with three different models. (b) Experimental rate constants. (c) Efficiencies $\Phi_{HSA} = k_{abs} / k_{HSA}$ (triangle), $\Phi_{ADO} = k_{abs} / k_{ADO}$ (circle) and $\Phi_{SCC} = k_{abs} / k_{SCC}$ (diamonds).

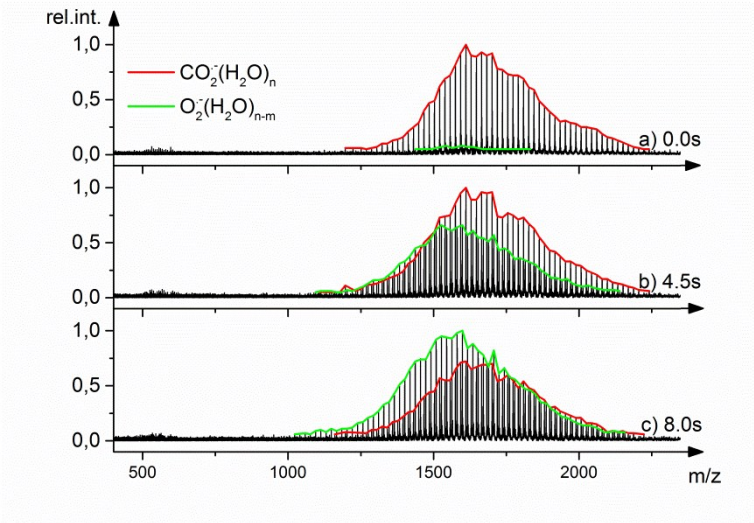

Figure S4: Mass spectra of the reaction $CO_2^{\bullet-}(H_2O)_n$ with O_2 at 0.0s, 4.5s and 8.0s at T = 120 K and $p(O_2) = 9.5 \cdot 10^{-9}$ mbar. a) At the beginning of the reaction the reactant clusters are the dominant species. b) After 4.5s the product clusters distribution is increased almost to the same quantity as the reactant clusters. c) At 8s the charge transfer is still not completed and nearly three-quarters of the clusters changed the core to $O_2^{\bullet-}(H_2O)_{n-m}$.

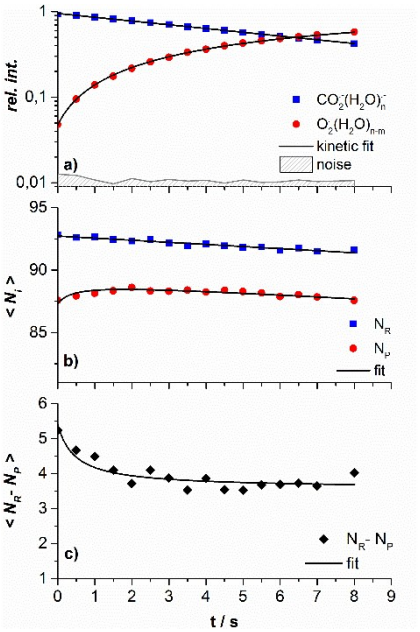

Figure S5: a) kinetics and (b and c) nanocalorimetric fits of reaction (5), $CO_2^{\bullet-}(H_2O)_n$ with O_2 at T = 120 K and $p(O_2) = 9.5 \cdot 10^{-9}$ mbar. Blue filled square, $CO_2^{\bullet-}(H_2O)_n$; red filled circle, $O_2^{\bullet-}(H_2O)_{n-m}$; filled diamond, difference in the cluster size.

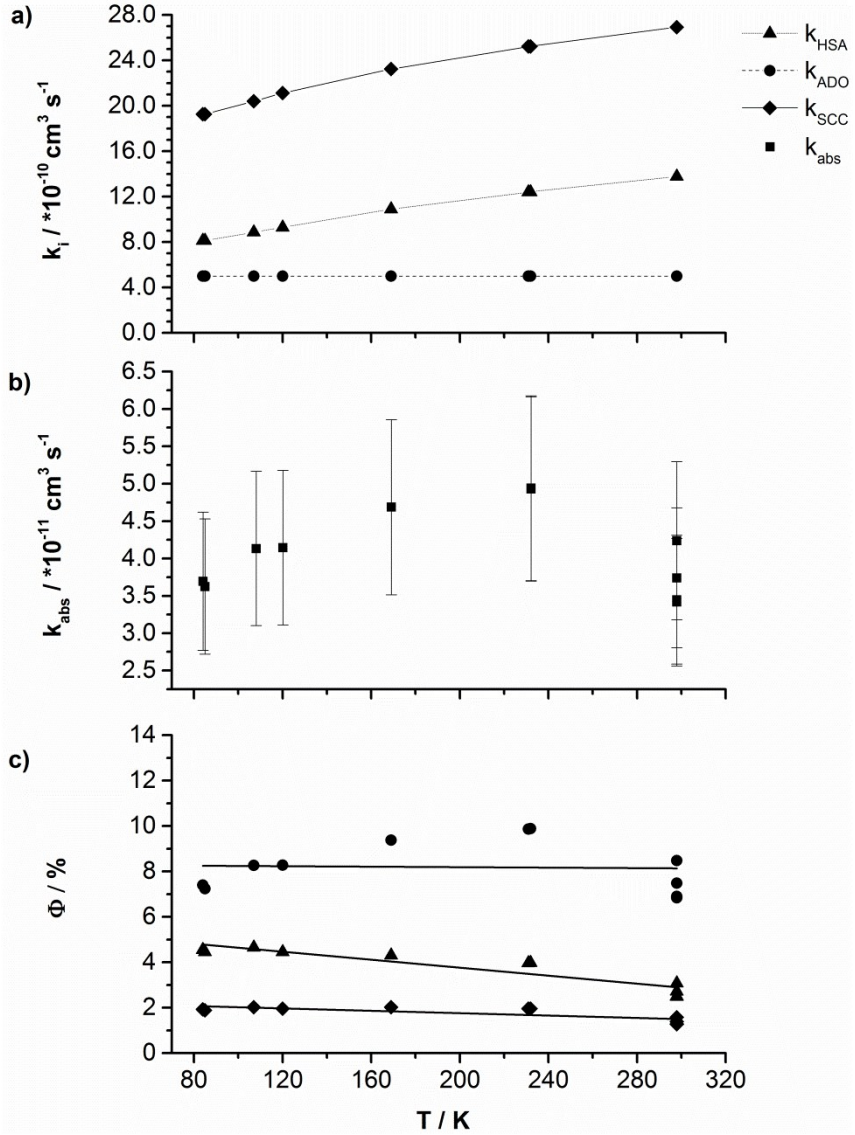

Figure S6: Kinetic analysis of reaction (5). (a) Calculated collision rates with three different models. (b) Experimental rate constants. (c) Efficiencies $\Phi_{HSA} = k_{abs} / k_{HSA}$ (triangle), $\Phi_{ADO} = k_{abs} / k_{ADO}$ (circle) and $\Phi_{SCC} = k_{abs} / k_{SCC}$ (diamonds).

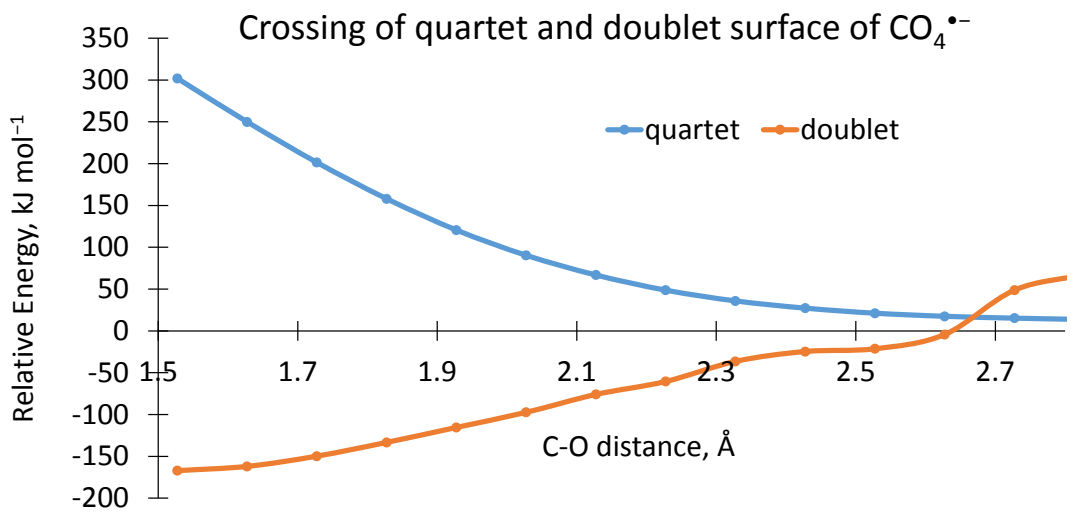

Figure S7: Energy scan for the O_2C—O_2 distance of $CO_4^{\bullet-}(H_2O)_5$ (with a fixed bent OCO angle) at the quartet and doublet surfaces.

Table S1: Relative energy of $CO_2^{\bullet-}(H_2O)_{10}$ optimized at M06-2X/6-311++G(d,p) level.

	$CO_2^-(H_2O)_{10}$	ΔE_{zpc}
r10-a	fused cubic structures	0.0
r10-b		5.8
r10-c		8.5
r10-d	less-ordered liquid-like structures	21.3
r10-e		22.7
r10-f		27.1
r10-g		30.6
r10-h		31.8
r10-i		34.1
r10-j		34.6
r10-k		34.9
r10-l		38.3
r10-m		39.1
r10-n		42.2
r10-o		45.6
r10-p		51.1

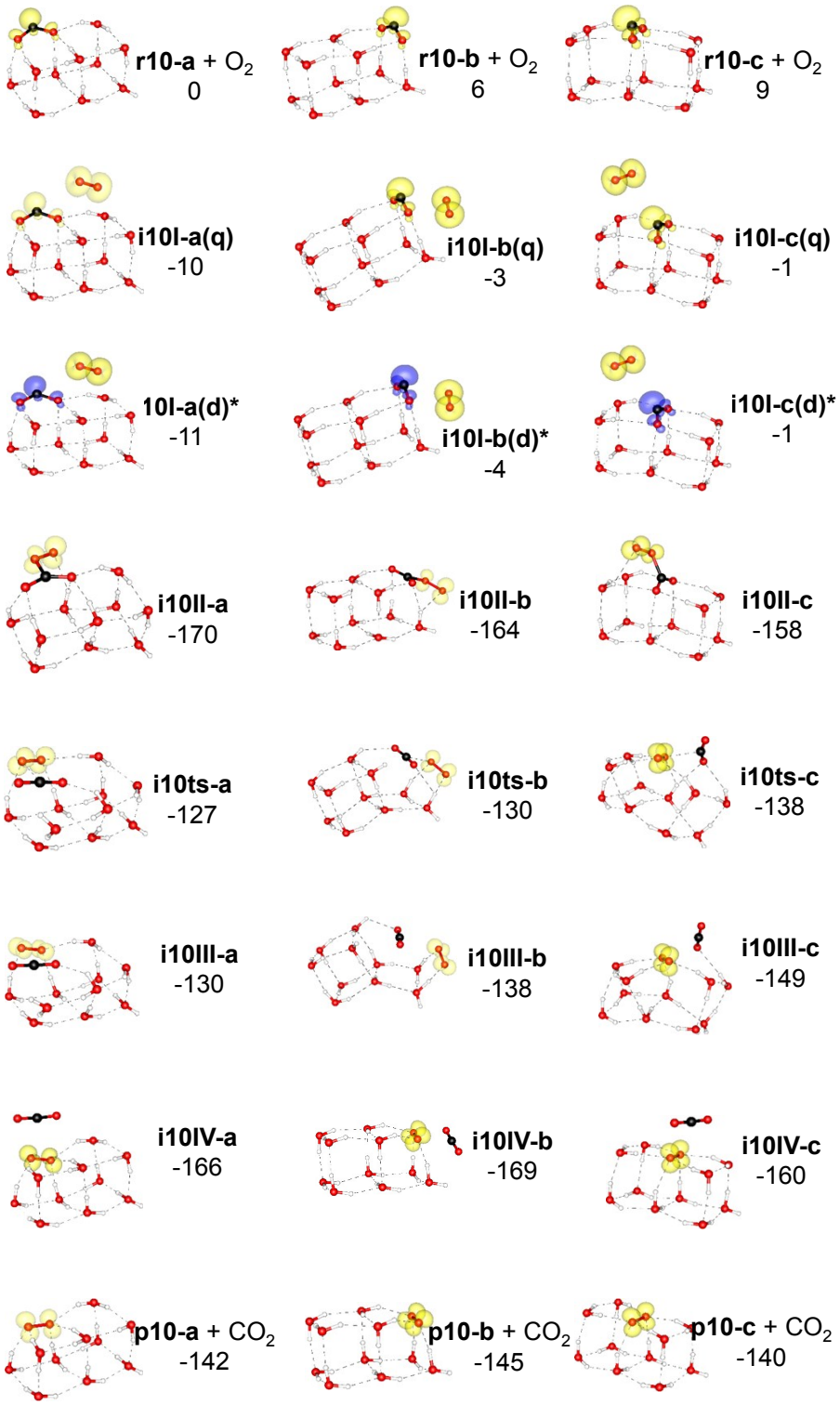

Figure S8: Geometries for the exchange reaction $CO_2^{\bullet-}(H_2O)_{10} + O_2 \rightarrow O_2^{\bullet-}(H_2O)_{10} + CO_2$. **The spin distributions of the doublet **i10I-x(d)** were obtained from single-point calculations on the geometries of the quintet **i10I-x(q)**. The spin densities were plotted with iso-values of 0.02 (yellow) and -0.02 (blue).

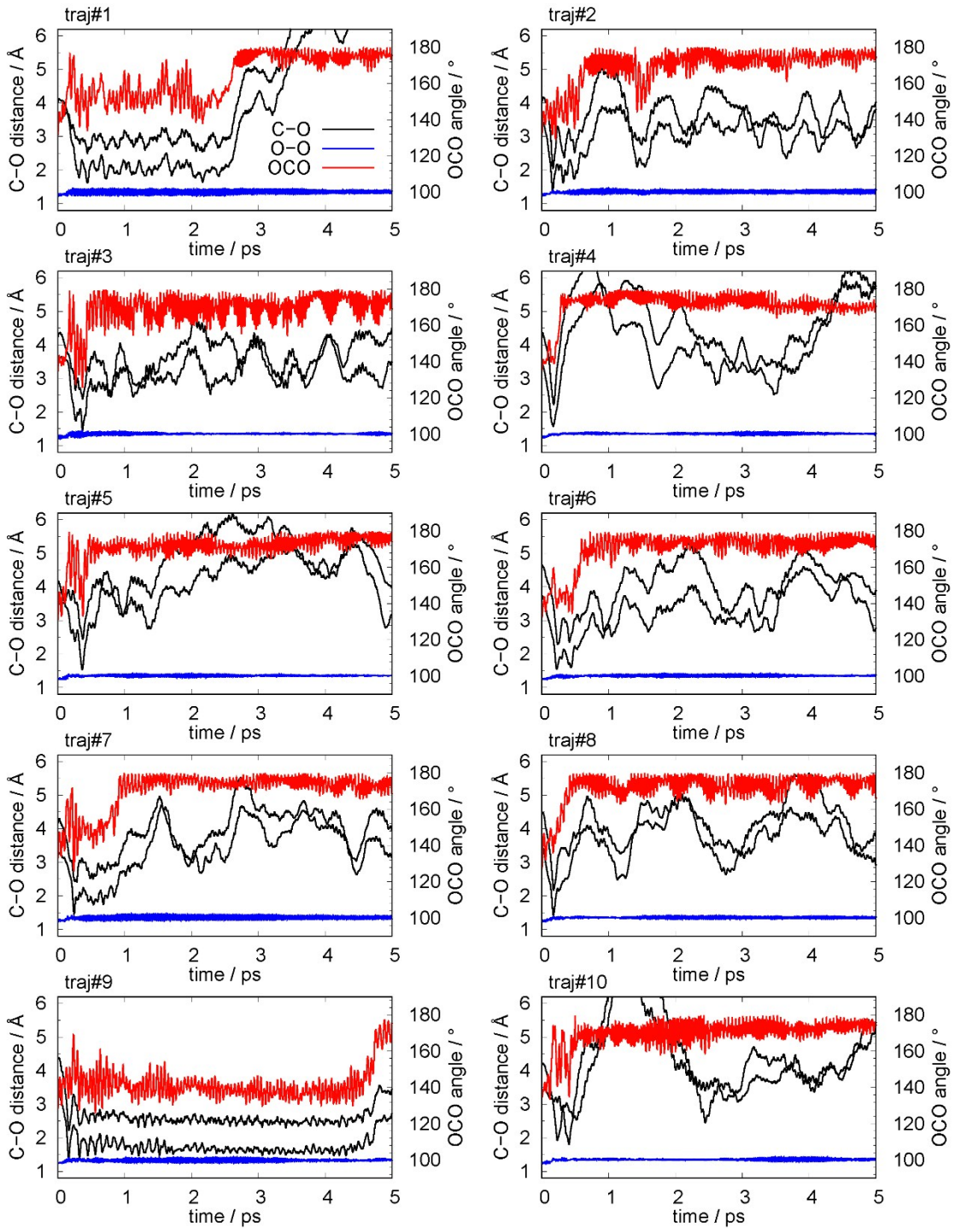

Figure S9: Ten DFT-MD trajectories simulated under the NVE conditions for the exchange reaction $CO_2^{\bullet-}(H_2O)_{10} + O_2 \rightarrow O_2^{\bullet-}(H_2O)_{10} + CO_2$. The two C-O distances between the C atom of CO_2 and the two O atoms of O_2 (black), the O-O distance of O_2 (blue) and the OCO angle of CO_2 (red). The traj#8 (with 0 – 2 ps) is shown in Figure 6 of the main text.

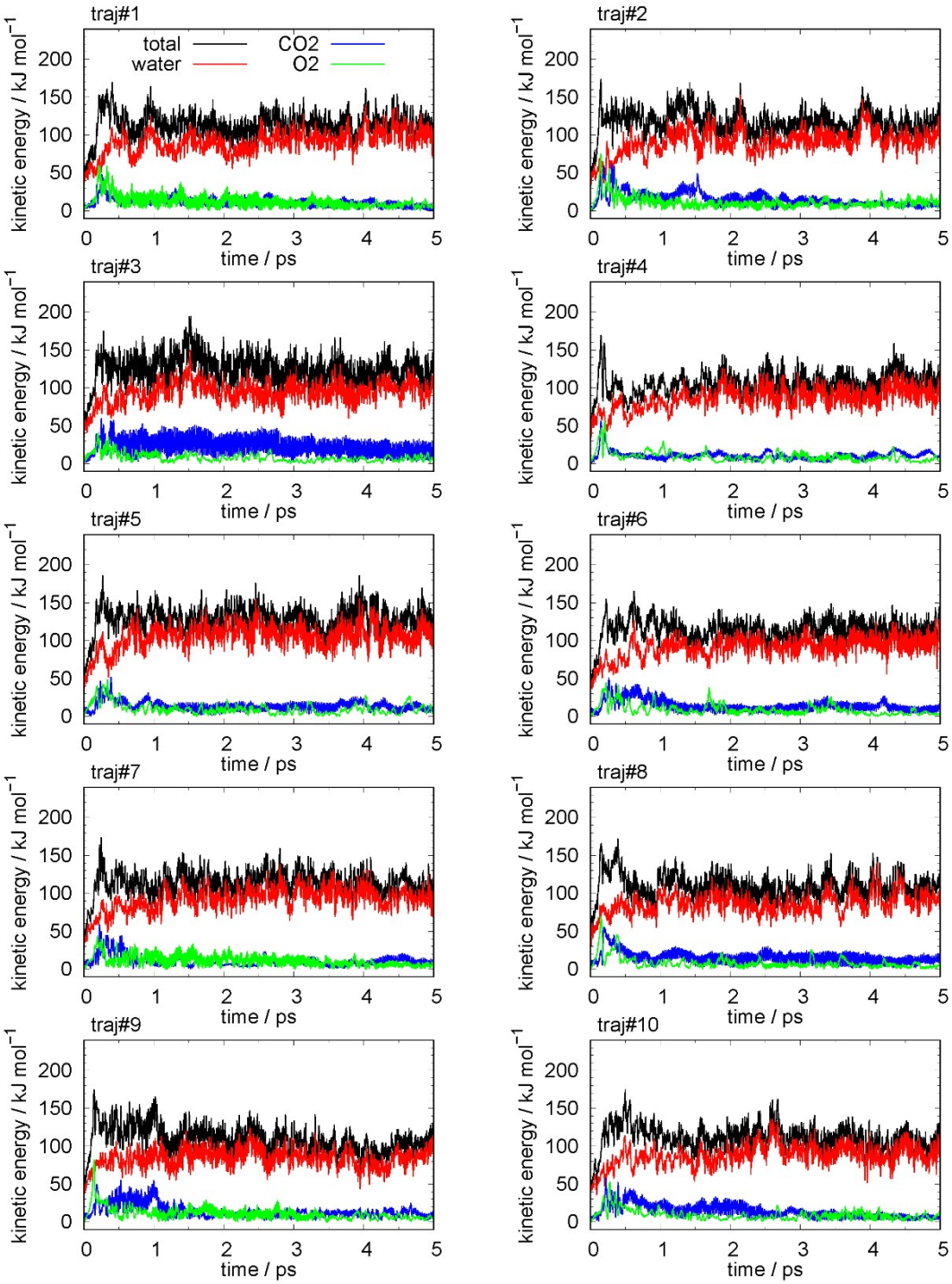

Figure S10: Ten respective DFT-MD trajectory simulated under the NVE conditions for the exchange reaction $CO_2^{\bullet-}(H_2O)_{10} + O_2 \rightarrow O_2^{\bullet-}(H_2O)_{10} + CO_2$. The kinetic energies of the entire system (black) and the sub-systems, including the water cluster (red), CO_2 (blue) and O_2 (green), determined from the atomic velocities of the respective systems. The traj#8 (with 0 – 2 ps) is shown in Figure 6 of the main text.

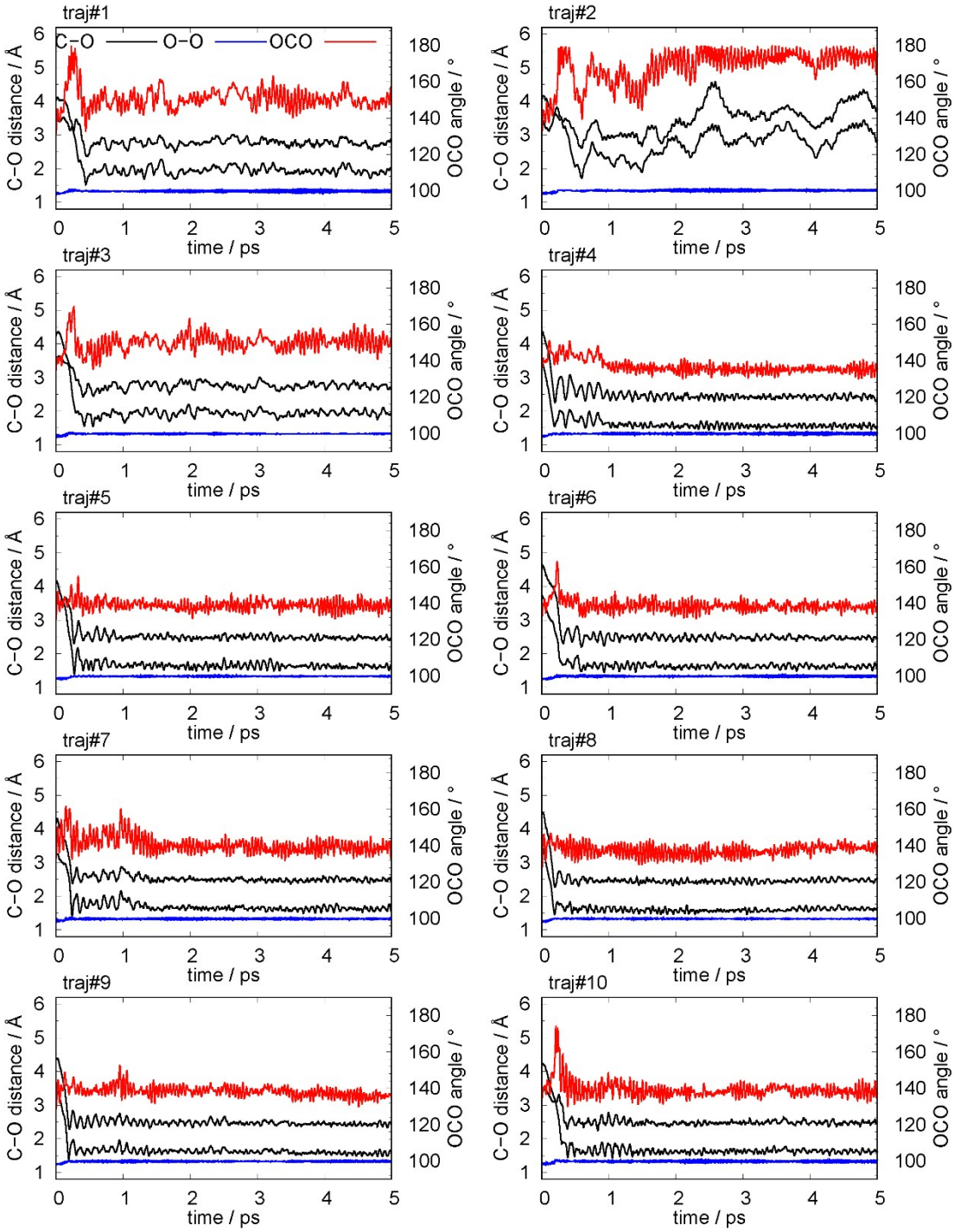

Figure S11: Ten DFT-MD trajectories simulated under the NVT conditions at 100 K for the reaction $CO_2^{\bullet-}(H_2O)_{10} + O_2$. The two C-O distances between the C atom of CO_2 and the two O atoms of O_2 (black), the O-O distance of O_2 (blue) and the OCO angle of CO_2 (red). An intact $CO_4^{\bullet-}$ was formed for all trajectories, except traj#2.

Table S2: Cartesian coordinates for the stationary structures shown in **Figures 4**, **5** and **S8**.

18
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H 0.175079 1.831481 0.727658
H -1.161405 1.824673 -0.033246
H -2.321803 0.010837 -0.761450
H -2.337223 0.026743 0.723280
H 0.392152 -0.025904 1.952503
H 1.767372 0.339088 1.423921
H 0.625860 1.305993 -1.397591
H 0.418288 -0.097875 -1.949327
H 2.011438 -1.394331 0.043824
H 2.267358 -0.138979 -0.761863
O -0.272315 2.214787 -0.048020
O -2.642900 0.557751 -0.028256
O 1.042714 0.693163 1.966571
O 1.059476 0.628630 -1.951088
O 2.626137 -0.650191 -0.010291
O -0.851807 -1.393101 -1.110341
O -0.864711 -1.330943 1.160877
C -0.434980 -1.573747 0.032778

20
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H 1.877638 1.132879 -1.242471
H 1.067529 2.257058 -0.623402
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H -0.826334 -0.309832 1.097348
H -0.977040 1.521726 -1.148835
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O 2.212269 -2.080694 0.452232
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O -0.775192 0.468124 1.673631
O -0.865914 2.236820 -0.508539
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H 1.229053 1.316993 1.398574
H 0.036348 1.435415 -1.472894
H 0.523970 0.030225 -1.840557
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H 2.105665 1.127284 -0.615404
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O 2.675225 1.106339 0.182392
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O -1.022842 -1.110480 1.285839
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H 2.977574 0.301703 0.361198
H 2.712018 -1.025094 -0.302257
H 0.454840 0.293260 -1.722317
H -0.614466 1.381778 -1.434756
H 0.120980 1.300899 1.588071
H -0.784065 0.082312 1.823143
H -2.727300 0.920962 -0.630534
H -1.801484 1.582118 0.370361
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O -0.794279 1.051493 1.791863
O -2.212521 1.725834 -0.506490
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H 0.652449 -0.365581 1.467733
H 2.084230 -0.910957 1.443167
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O 1.296963 -0.044409 0.159286
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H 0.029679 -0.228348 1.609404
H 1.274763 0.601666 1.610475
H 0.247895 1.401681 -1.330599
H 0.557837 -0.026120 -1.738160
H 1.974568 -0.909828 0.271562
H 2.248771 0.375237 -0.477051
O -1.093340 1.961723 -0.073603
O -2.591280 -0.484808 0.010928
O 0.369623 0.610777 1.963175
O 0.916245 0.875077 -1.803164
O 2.568941 -0.137986 0.283757
O 0.198350 -1.663877 0.339264
O -0.318503 -1.467696 -0.850370

33
r10-a: E=-953.011068531 Ezpc=-952.740108
H 0.283676 -1.392997 0.800073
H 1.363815 -2.219250 0.047294
H 3.996475 -2.251900 -0.231575
H 3.146590 -1.045075 -0.781262
H -0.159473 0.716530 1.233620
H -1.025626 -0.200086 2.113373
H -2.967611 0.316795 1.342309
H -2.782436 -1.210088 1.330702
H 1.759619 0.027282 2.251787
H 2.937888 -0.563462 1.453875
H 1.943675 0.065449 -2.132471
H 2.805104 0.978415 -1.259064

H 1.463803 2.365513 -0.001849
H 2.540788 1.621125 0.820124
H 0.124265 -0.856170 -1.301141
H -0.085513 0.665319 -1.347770
H -2.637208 -1.849027 -0.776581
H -1.481204 -2.565287 -0.054483
H -2.945422 0.353778 -1.347066
H -1.875689 -0.295956 -2.213302
O 0.411591 -2.036545 0.071923
O 3.202544 -1.741180 -0.066250
O -0.092348 -0.025351 1.862671
O -2.786208 -0.435722 1.925248
O 2.689821 0.179719 2.023735
O 2.859144 0.176589 -1.822171
O 2.412067 2.165021 0.022485
O 0.049961 -0.108735 -1.925457
O -2.438378 -2.428970 -0.018608
O -2.798814 -0.403456 -1.934722
O -0.426312 1.998756 -0.092492
O -2.676009 1.788737 -0.001231
C -1.610330 2.384697 -0.051272

35
i10I-a(q): E=-1103.324190330 Ezpc=-1103.048506
H -0.107582 -1.141252 -1.425152
H -1.076678 -2.349815 -1.325525
H -3.691061 -2.755634 -1.158284
H -2.908936 -2.067770 0.021759
H 0.134660 0.814881 -0.479133
H 1.016020 0.747246 -1.738729
H 2.935124 0.954414 -0.815356
H 2.898829 -0.292071 -1.716494
H -1.779927 0.773263 -1.687066
H -2.854557 -0.299630 -1.440816
H -1.737399 -1.895865 1.787088
H -2.722489 -0.734598 1.644728
H -1.600178 1.270353 1.519739
H -2.648989 1.066989 0.409594
H 0.108609 -1.931422 0.585268
H 0.170741 -0.720013 1.531403
H 2.920780 -2.077482 -0.412585
H 1.803385 -2.355183 -1.434934
H 3.053580 -0.639882 1.367128
H 2.101333 -1.791140 1.660390
O -0.145261 -2.099924 -1.222787
O -2.943789 -2.185891 -0.969772
O 0.092291 0.612174 -1.432977
O 2.797197 0.678678 -1.734008
O -2.706752 0.657869 -1.425396
O -2.673901 -1.713959 1.597694
O -2.525465 1.019314 1.374923
O 0.154075 -1.694695 1.531920
O 2.735376 -2.104554 -1.369287
O 3.013074 -1.608344 1.383097
O 0.316335 1.136463 1.335265
O 2.564681 1.276575 1.139406
C 1.457892 1.587428 1.552722
O -1.188259 3.176703 -0.409636
O -0.084928 3.587097 -0.574613

35
i10II-a: E=-1103.388761300 Ezpc=-1103.109390
H -0.699330 -1.666281 -0.150357
H -1.815032 -1.649152 0.944894
H -4.407719 -1.452407 1.376356
H -3.461393 -0.202928 1.210046
H 0.059396 -0.751227 -1.875303
H 0.585687 -2.183744 -1.772292
H 2.607941 -1.573374 -1.156592
H 2.160477 -2.670652 -0.191010
H -2.127560 -1.310826 -2.001234
H -3.267093 -1.067214 -0.982956
H -2.073773 1.273614 1.967795
H -2.689562 1.643370 0.627644
H -1.096988 1.812209 -1.161543
H -2.345812 0.960167 -1.447797
H -0.332331 0.071478 1.278493
H -0.095296 1.559378 0.920182
H 2.086710 -1.759372 1.907192
H 0.742997 -2.387972 1.529500
H 2.969755 0.245799 1.226245
H 1.745615 0.503012 2.105573
O -0.856748 -1.577351 0.813722
O -3.625599 -1.141341 0.918550
O -0.248261 -1.677436 -1.859128
O 2.272752 -2.483501 -1.142239
O -2.922837 -0.780865 -1.841437
O -2.934130 1.325547 1.524665
O -2.056497 1.789006 -1.024444
O -0.096048 0.940680 1.663284
O 1.686630 -2.593660 1.604007
O 2.601242 0.042992 2.096673
O 0.620475 0.890137 -1.376184
O 2.760724 0.361820 -0.850306
C 1.748618 1.034192 -0.929008
O 1.996519 2.385024 -0.296741
O 0.921978 3.069070 -0.078021

35
i10ts-a: E=-1103.367789000 Ezpc=-1103.092868 (TS freq=306i)
H -0.599239 -1.918528 0.596801
H -1.749480 -1.387806 1.494533
H -4.377651 -1.245317 1.533348
H -3.528997 -0.025152 0.985249
H 0.139931 -1.905696 -1.385545
H 0.912127 -3.031566 -0.729931
H 3.326796 -2.340851 -0.640046
H 2.498066 -2.162225 0.645821
H -1.918037 -2.332339 -1.378162
H -2.990084 -1.505025 -0.646841
H -2.405064 1.686405 1.132443
H -3.009691 1.546115 -0.244548
H -1.137858 1.601181 -1.623731
H -1.950491 0.277557 -1.789346
H -0.541910 0.523055 1.148034
H -0.279392 1.897215 0.430139
H 2.208500 -0.098210 1.853590
H 1.028270 -1.101669 1.969281
H 2.288520 2.080720 0.862823
H 1.230633 1.807248 1.904625
O -0.785045 -1.382751 1.386365
O -3.555266 -1.025839 1.093335
O 0.006941 -2.775422 -0.988649
O 2.641892 -2.766168 -0.118851
O -2.519138 -1.587039 -1.491293
O -3.264930 1.515594 0.700925
O -2.030822 1.243028 -1.750695
O -0.568193 1.483958 1.289507
O 1.989615 -1.051405 1.860035
O 2.186860 1.713933 1.756742
O 0.793168 -0.038646 -1.006891
O 3.091530 0.207490 -0.951108
C 1.932603 0.193668 -0.961618
O 1.601898 2.518022 -0.941986
O 0.318922 2.754354 -0.881038

35
i10III-a: E=-1103.369480130 Ezpc=-1103.094294
H 0.515340 1.868541 0.676283
H 1.703216 1.356340 1.527349
H 4.331048 1.352115 1.519685
H 3.545925 0.114334 0.914247
H -0.249175 2.052620 -1.328888
H -1.028366 3.082397 -0.541133
H -3.576851 2.454550 -0.304764
H -2.574384 1.975840 0.781843
H 1.807713 2.479030 -1.276866
H 2.912863 1.628950 -0.634568
H 2.547728 -1.651401 1.038469
H 3.065365 -1.414334 -0.370679
H 1.212018 -1.557793 -1.745949
H 1.910207 -0.156927 -1.845788
H 0.635813 -0.630000 1.300482
H 0.419665 -1.996105 0.562444
H -2.172333 -0.186791 1.764236
H -1.070922 0.889580 1.986667
H -1.996532 -2.277892 0.636998
H -1.163838 -2.050321 1.895056
O 0.736344 1.319309 1.446625
O 3.516904 1.110210 1.076210
O -0.124125 2.871014 -0.833898
O -2.729479 2.663979 0.091462
O 2.412090 1.750193 -1.457009
O 3.368267 -1.411634 0.562253
O 2.071582 -1.111833 -1.850398
O 0.756200 -1.586684 1.411856
O -2.024214 0.780031 1.853342
O -2.066711 -1.942563 1.563236
O -0.959446 0.173843 -1.134574
O -3.213485 -0.292688 -0.925248
C -2.079669 -0.095842 -1.017301
O -1.416324 -2.598493 -0.993575
O -0.114665 -2.569393 -0.866698

35
i10IV-a: E=-1103.385350040 Ezpc=-1103.107798
H -1.014696 0.780221 1.379418
H -2.497186 1.198685 1.289927
H -4.844139 -0.043137 1.047523
H -3.735674 -0.150097 -0.064352
H 0.292449 -0.710312 0.572206
H 0.956298 -0.206299 1.855959
H 2.685911 0.659073 0.865777
H 1.973029 1.696638 1.730595
H -1.308040 -1.795440 1.817027
H -2.786499 -1.562905 1.471749
H -2.695179 0.468072 -1.810180
H -2.633562 -1.055707 -1.606047
H -0.497143 -1.873965 -1.235271
H -1.563028 -2.462425 -0.279114
H -1.427419 1.821524 -0.672344
H -0.574101 0.991245 -1.616798
H 1.034464 3.149694 0.329022
H -0.067060 2.795543 1.351681
H 1.693492 1.962726 -1.453888
H 0.446378 2.777772 -1.795176
O -1.596710 1.545089 1.193560
O -3.894526 -0.065528 0.919710
O 0.125139 -0.603662 1.527792
O 2.452048 0.845524 1.784446
O -2.110378 -2.255119 1.524161

O -3.259279 -0.301072 -1.609731
O -1.374663 -2.284854 -1.217963
O -1.272932 1.684244 -1.623994
O 0.857608 3.071333 1.285873
O 1.351868 2.878046 -1.470149
O 2.007866 -2.553171 -0.212213
O 4.056668 -1.486249 -0.133465
C 3.007888 -1.973978 -0.189864
O 1.861037 0.156032 -1.048232
O 0.610550 -0.205244 -1.174610

32
p10-a: E=-914.801002899 Ezpc=-914.536053
H -0.113494 0.722165 -1.266898
H -1.132242 -0.096639 -2.096385
H -3.765919 -0.432051 -2.267298
H -2.973344 -0.870866 -0.980140
H 0.228828 1.354307 0.717980
H 0.993220 2.345490 -0.167390
H 2.741990 1.599553 0.705181
H 2.924207 1.452921 -0.798241
H -1.741193 2.292362 -0.079992
H -2.866296 1.410255 -0.655179
H -1.825035 -2.191251 0.218353
H -2.631518 -1.206284 1.062603
H -1.198481 0.223244 2.224484
H -2.378438 0.941068 1.529969
H 0.022789 -1.542097 -0.729744
H 0.245365 -1.542918 0.770406
H 2.873035 -0.816645 -1.236337
H 1.773253 -0.167568 -2.098861
H 2.735809 -1.373040 0.893513
H 2.047680 -2.459880 0.081632
O -0.193417 -0.054324 -1.858259
O -3.009332 -0.204940 -1.724646
O 0.093911 1.996772 -0.014208
O 2.841498 2.130513 -0.101906
O -2.669818 2.040934 0.053496
O -2.726601 -1.831611 0.315452
O -2.159493 0.195276 2.119084
O 0.032833 -2.153206 0.029683
O 2.704771 -0.081519 -1.854449
O 2.907043 -2.029127 0.190501
O 1.989220 0.104441 1.733356
O 0.694357 -0.068477 1.633439

33
r10-b: E=-953.008513674 Ezpc=-952.737889
H -0.586021 -1.686991 1.670651
H 0.319682 -0.451603 1.581339
H 0.063613 1.445125 0.421593
H -0.890763 1.450732 1.620266
H -2.639291 -0.721259 1.520006
H -2.604201 -1.876635 0.533713
H 0.276013 -1.560648 -0.288008
H -0.759736 -1.717734 -1.433774
H -2.768758 -0.545748 -1.304736
H -3.308710 -1.809815 -2.040043
O 0.339077 -1.424924 1.503359
O 0.046599 1.353275 1.394340
O -2.426009 -1.669073 1.462014
O 0.164094 -1.479976 -1.257959
O -2.651432 -1.524015 -1.402827
O -2.917364 1.125401 -1.053691
O -2.836309 1.158491 1.211079
C -3.073829 1.585854 0.086499
O 2.906730 1.446095 1.406511
H 1.990660 1.549480 1.696625
H 3.081412 0.487019 1.461572
O -0.057272 1.286860 -1.406905
H -1.007817 1.428192 -1.533267
H 0.060162 0.317691 -1.464493
O 2.776305 1.638787 -1.391954
H 1.836340 1.811889 -1.536579
H 2.893912 1.704227 -0.425078
O 3.165556 -1.344104 1.215094
H 3.203309 -1.396332 0.241457
H 2.279022 -1.657506 1.441755
O 2.983463 -1.155180 -1.589056
H 2.062613 -1.397642 -1.755678
H 2.994024 -0.180664 -1.646367

35
i10I-b(q): E=-1103.321292890 Ezpc=-1103.045988
H -0.171868 -1.789644 1.383879
H 0.801424 -0.609428 1.486463
H 0.724557 1.414255 0.543673
H -0.311883 1.355128 1.672317
H -2.140464 -0.665304 1.227340
H -2.096707 -1.697119 0.114566
H 0.841062 -1.506302 -0.499675
H -0.103556 -1.475829 -1.730742
H -2.059482 -0.192812 -1.570403
H -2.669990 -1.358857 -2.402450
O 0.774209 -1.567305 1.297911
O 0.631063 1.217771 1.496585
O -1.996643 -1.615833 1.074523
O 0.812919 -1.311624 -1.459326
O -1.978480 -1.159098 -1.768378
O -2.138908 1.456097 -1.151154
O -2.244784 1.240986 1.102039
C -2.354110 1.805086 0.017974
O -4.538696 -0.412400 -0.240559
O -4.986800 -0.213204 0.842000
O 3.485114 1.148779 1.712257
H 2.556447 1.273700 1.948852
H 3.606027 0.180807 1.670385
O 0.741128 1.462390 -1.291983
H -0.187930 1.675077 -1.468595
H 0.813118 0.501194 -1.457136
O 3.578687 1.655610 -1.048321
H 2.660462 1.892056 -1.236633
H 3.625937 1.607382 -0.074511
O 3.616498 -1.614279 1.224664
H 3.726115 -1.560676 0.256461
H 2.701718 -1.901560 1.351157
O 3.661902 -1.107911 -1.543802
H 2.746328 -1.277225 -1.803752
H 3.725675 -0.135204 -1.490687

35
i10II-b: E=-1103.386488730 Ezpc=-1103.107242
H 0.094559 0.941849 2.129957
H -0.797877 -0.171678 1.548383
H -0.706057 -1.508131 -0.194910
H 0.311326 -2.003251 0.847320
H 2.343220 0.194485 2.024285
H 2.122397 1.446159 1.156555
H -0.767359 1.574901 0.225063
H 0.218046 2.214483 -0.786341
H 2.277847 1.122926 -1.128688
H 2.981981 2.468440 -0.902316
O -0.812662 0.767035 1.824202
O -0.628296 -1.778228 0.740129
O 1.960337 1.079784 2.040583
O -0.682649 1.869501 -0.705833
O 2.161390 2.003774 -0.719667
O 2.168152 -0.699055 -1.228869
O 2.212067 -1.790181 0.759912
C 2.603218 -1.092427 -0.155414
O 4.474575 0.278191 -0.652244
O 3.983261 -0.563872 0.196573
O -3.487047 -1.832859 0.817658
H -2.568364 -2.052016 1.023105
H -3.631487 -0.956300 1.222782
O -0.579080 -0.686183 -1.835146
H 0.379170 -0.834048 -1.877613
H -0.663281 0.246615 -1.558788
O -3.413353 -0.996870 -1.863979
H -2.479622 -1.122149 -2.080292
H -3.519397 -1.405805 -0.983968
O -3.651854 0.840300 1.661502
H -3.709461 1.243514 0.774916
H -2.746191 1.020284 1.949498
O -3.527805 1.680421 -1.021809
H -2.610360 1.964849 -1.128280
H -3.564676 0.795372 -1.432275

35
i10ts-b: E=-1103.370510560 Ezpc=-1103.094280 (TS freq=242i)
H 0.413110 0.674080 2.027957
H -0.701246 -0.354042 1.631848
H -1.006223 -1.810284 -0.084934
H -0.165555 -2.450668 1.031080
H 2.825682 0.377388 1.752421
H 2.252809 1.606905 1.073562
H -0.393643 1.225393 0.122806
H 0.640433 1.638174 -0.967557
H 3.128836 1.324891 -0.877426
H 2.828415 2.857135 -1.058117
O -0.533406 0.589270 1.799023
O -1.021947 -2.040446 0.865036
O 2.167271 1.075258 1.880938
O -0.293787 1.388969 -0.837272
O 2.411553 2.027298 -0.818928
O 2.061819 -0.838744 -1.370990
O 1.899301 -2.024788 0.615905
C 2.119047 -1.362139 -0.327063
O 4.377510 0.383530 -0.421411
O 3.933620 -0.574311 0.332656
O -3.805487 -1.313599 0.979468
H -2.969038 -1.750030 1.184782
H -3.707858 -0.407390 1.332697
O -0.843163 -1.079523 -1.747364
H -0.053620 -1.376720 -2.209680
H -0.634730 -0.146353 -1.497579
O -3.677920 -0.642675 -1.743854
H -2.797724 -0.972507 -1.968327
H -3.835701 -0.971239 -0.838381
O -3.271584 1.339372 1.671830
H -3.276230 1.716353 0.772027
H -2.335718 1.303197 1.915622
O -3.081379 2.023423 -1.053151
H -2.122910 2.016557 -1.184232
H -3.382576 1.167718 -1.411265

35
i10III-b: E=-1103.372208730 Ezpc=-1103.097354
H 0.412870 1.017357 1.854499
H -0.766541 -0.032388 1.767590
H -1.227200 -1.893007 0.461724

H -0.651992 -2.312226 1.820650
H 2.747934 0.730090 1.445332
H 2.164531 1.973981 0.830663
H -0.210350 0.978771 -0.102643
H 0.929786 1.138299 -1.170774
H 3.374790 1.151474 -0.900796
H 2.808478 2.388092 -1.786467
O -0.543814 0.904233 1.657728
O -1.393160 -1.848010 1.422258
O 2.099839 1.440928 1.636515
O 0.001189 0.832235 -1.047429
O 2.536828 1.762148 -1.113532
O 2.136498 -1.576055 -1.201669
O 1.493917 -1.656897 1.016853
C 1.853628 -1.580511 -0.082026
O 4.439508 0.299366 -0.472407
O 3.980603 -0.307926 0.591373
O -4.020765 -0.674521 1.137838
H -3.259524 -1.141971 1.503807
H -3.801423 0.274112 1.231254
O -0.864422 -1.637614 -1.317327
H -0.310333 -2.163937 -1.898616
H -0.484711 -0.718577 -1.333294
O -3.628584 -0.836720 -1.631762
H -2.775474 -1.290970 -1.638380
H -3.904045 -0.856984 -0.695377
O -3.112898 1.959529 1.114585
H -3.012930 2.072154 0.151430
H -2.207037 1.836245 1.435064
O -2.646487 1.810931 -1.667874
H -1.699040 1.613749 -1.685316
H -3.075570 0.945781 -1.799385

35
i10IV-b: E=-1103.386990450 Ezpc=-1103.109038
H 0.296707 0.189235 -2.097829
H -0.655786 0.914043 -1.111426
H -0.980032 1.190733 1.064786
H 0.298518 1.892049 0.611784
H 2.172337 0.423182 -1.048579
H 2.154295 -1.005941 -1.539662
H -0.813966 -1.262734 -0.837898
H 0.004979 -2.383889 -0.157005
H 1.936346 -1.471674 0.595857
H 2.732608 -2.745030 0.167471
O -0.636366 0.246077 -1.824683
O -0.662698 1.876780 0.450046
O 2.155458 -0.096224 -1.874079
O -0.880792 -1.990622 -0.187176
O 1.928219 -2.257930 -0.021319
O 4.424571 -0.612462 0.352440
O 4.677473 1.595945 -0.278253
C 4.509812 0.498820 0.040471
O 1.624075 -0.085861 1.409186
O 1.951946 0.963486 0.699701
O -3.459413 2.198514 -0.065702
H -2.525380 2.437318 -0.005522
H -3.525435 1.644149 -0.867455
O -1.034140 -0.383453 2.107136
H -0.079424 -0.232359 2.220975
H -1.065942 -1.040605 1.385959
O -3.819722 0.132636 1.814651
H -2.937990 0.061682 2.205112
H -3.779936 0.931069 1.255136
O -3.455356 0.310050 -2.135657
H -3.650367 -0.477511 -1.593708
H -2.509984 0.237428 -2.329441
O -3.741280 -1.767381 -0.259986
H -2.847443 -2.127061 -0.179684
H -3.858768 -1.203442 0.527847

32
p10-b: E=-914.802082355 Ezpc=-914.537005
H 1.156625 -1.476654 -1.459169
H 0.055214 -0.377743 -1.478858
H -0.386914 1.596907 -0.532047
H 0.764361 1.665966 -1.528432
H 3.016380 -0.377031 -1.339134
H 3.201483 -1.551305 -0.402466
H 0.247578 -1.277199 0.513882
H 1.258137 -1.166903 1.677978
H 2.967623 0.134811 1.074728
H 3.807656 -0.693075 2.128190
O 0.207944 -1.322316 -1.286105
O -0.187768 1.460127 -1.475267
O 2.998616 -1.354883 -1.327274
O 0.310142 -1.109676 1.476640
O 3.124117 -0.783779 1.462751
O 2.444827 1.453282 0.367737
O 2.513448 1.340164 -0.934774
O -2.972058 0.843027 -1.602660
H -2.099567 1.121714 -1.910116
H -2.914195 -0.130095 -1.536964
O -0.133773 1.656667 1.349996
H 0.780489 1.915452 1.137433
H -0.052614 0.698952 1.522147
O -2.966325 1.368587 1.164064
H -2.092248 1.760007 1.297032
H -3.064178 1.297122 0.195659
O -2.564490 -1.878667 -1.078537
H -2.630270 -1.839675 -0.106032
H -1.616265 -1.967902 -1.251873
O -2.531372 -1.364381 1.691283
H -1.587189 -1.381494 1.899727
H -2.758578 -0.417071 1.635480

33
r10-c: E=-953.006898955 Ezpc=-952.736843
H -3.034221 0.533625 -1.371044
H -3.655984 1.894624 -1.863609
H 2.808423 1.828171 -0.329357
H 1.670564 1.875137 -1.366925
H -1.942606 -1.327217 -1.513971
H -2.990555 -1.334197 -0.396980
H -1.898514 -1.641734 1.455555
H -2.920617 -0.504330 1.609209
H 2.082477 -1.273454 -1.831034
H 2.920609 0.001223 -1.634747
H 1.973696 1.555095 1.759072
H 3.117970 0.583580 1.503701
H 2.269970 -1.631614 1.382798
H 3.173321 -1.280763 0.199456
H -1.115510 1.609044 -1.377349
H -0.169613 0.380628 -1.349288
H -1.827448 1.441047 1.744520
H -2.921825 1.597032 0.674698
H 0.072354 0.156529 1.562781
H 0.038709 1.331207 0.600452
O -2.992797 1.525933 -1.278129
O 2.629286 1.774082 -1.287350
O -2.868265 -1.091615 -1.340319
O -2.845157 -1.449437 1.381097
O 2.977354 -0.974534 -1.629244
O 2.907540 1.535260 1.502453
O 3.134350 -1.257954 1.175139
O -0.194259 1.346791 -1.218312
O -2.784786 1.353248 1.601901
O 0.053078 1.128444 1.555046
O -0.014483 -1.468054 -1.261886
O 0.045388 -1.690138 0.997053
C 0.328468 -1.941641 -0.172922

35
i10I-c(q): E=-1103.320305860 Ezpc=-1103.045107
H -3.285186 -0.777324 -1.480989
H -4.317122 0.051524 -2.335463
H 1.443895 2.958778 -0.776942
H 0.503517 2.293742 -1.798295
H -1.554759 -2.011163 -1.089314
H -2.656106 -2.171904 -0.036825
H -1.772029 -1.556684 1.839914
H -3.159820 -0.921026 1.667124
H 2.104190 -0.429375 -1.412183
H 2.398204 1.072305 -1.557937
H 0.542765 2.889738 1.306263
H 1.994370 2.424501 1.319427
H 2.137447 0.095542 1.799519
H 2.927280 0.491629 0.553254
H -1.946055 0.945699 -1.749834
H -0.613760 0.245052 -1.380677
H -2.910829 1.273084 1.285104
H -3.841263 0.709699 0.196830
H -0.659236 0.858874 1.502267
H -1.014831 1.640031 0.247583
O -3.641279 0.137173 -1.661359
O 1.411338 2.609096 -1.687729
O -2.514291 -2.136334 -1.007559
O -2.704947 -1.782568 1.706889
O 2.807373 0.222999 -1.299434
O 1.434661 3.180764 1.065262
O 2.784040 0.738876 1.486999
O -1.020735 1.121088 -1.513201
O -3.736225 0.776511 1.157274
O -1.041315 1.706986 1.220929
O 0.230238 -1.299399 -0.782831
O 0.074999 -0.932684 1.453696
C 0.593980 -1.289268 0.398510
O 3.374403 -2.584909 -0.585270
O 3.806172 -2.050987 0.385096

35
i10II-c: E=-1103.383771320 Ezpc=-1103.104990
H -3.413902 0.065414 -1.285618
H -4.377619 1.223677 -1.741535
H 1.952550 2.796917 -0.446862
H 0.803686 2.514376 -1.437495
H -1.880821 -1.469881 -1.518130
H -2.792392 -1.692979 -0.310202
H -1.541762 -1.615551 1.509369
H -2.843039 -0.812636 1.682472
H 2.095688 -0.448669 -1.966365
H 2.473870 1.019620 -1.673367
H 1.287528 2.411140 1.670518
H 2.639401 1.757503 1.415641
H 2.600186 -0.697510 1.458809
H 3.168315 -0.076437 0.176101
H -1.817834 1.557032 -1.358411
H -0.592982 0.600264 -1.341215
H -2.335307 1.321262 1.790800
H -3.474584 1.176904 0.764618
H -0.128737 0.563573 1.539449
H -0.556338 1.650075 0.573735

O -3.619820 1.034416 -1.186151
O 1.759553 2.655883 -1.393855
O -2.816560 -1.466917 -1.265551
O -2.503921 -1.696631 1.446201
O 2.812441 0.102116 -1.633883
O 2.187541 2.620851 1.381037
O 3.186440 0.002848 1.148472
O -0.856900 1.532362 -1.224800
O -3.243967 0.991679 1.686717
O -0.450397 1.480493 1.528947
O 0.035977 -1.121916 -1.286606
O 0.340436 -1.199790 0.955758
C 0.532941 -1.478355 -0.215837
O 1.588150 -2.478959 -0.487192
O 2.273083 -2.828181 0.554995

35
i10ts-c: E=-1103.373355760 Ezpc=-1103.097371 (TS freq=193i)
H 2.438878 -2.456431 -0.460636
H 1.901518 -3.917242 -0.691579
H -3.272478 -1.235181 -1.802580
H -1.787146 -1.159805 -2.150784
H 3.156899 -0.608543 -1.402790
H 3.197213 -0.583974 0.131411
H 1.907013 0.984443 1.487938
H 1.860928 -0.520193 1.862976
H -1.634151 1.528126 -0.682907
H -2.603926 0.803615 -1.644127
H -3.419943 -1.296107 0.598060
H -3.871127 -0.045443 -0.104730
H -1.399455 1.909118 1.822948
H -2.767475 1.771009 1.148321
H 0.362936 -1.862328 -0.857669
H 0.307428 -0.333006 -1.110748
H -0.078535 -1.724685 2.129419
H 1.037433 -2.570649 1.485664
H -1.886356 -0.144809 1.773939
H -1.226426 -0.876316 0.572498
O 1.673709 -3.067941 -0.310667
O -2.665105 -0.945477 -2.501594
O 3.446950 -1.133899 -0.649163
O 2.435960 0.170039 1.477519
O -2.580341 1.417662 -0.891183
O -4.094286 -0.983421 -0.025670
O -2.317335 1.611937 1.987344
O -0.246553 -1.120295 -1.008231
O 0.851570 -1.993322 2.238503
O -1.658196 -1.032539 1.431989
O 1.772101 0.965419 -1.868677
O 2.483041 2.633298 -0.443599
C 1.945139 1.797904 -1.047507
O 0.132725 1.685001 -0.083778
O 0.279001 1.987410 1.169758

35
i10III-c: E=-1103.377810880 Ezpc=-1103.101560
H -2.410245 2.546625 -0.651517
H -1.695102 3.846168 -1.169027
H 3.117390 0.893497 -2.105065
H 1.609012 0.739698 -2.284960
H -3.342030 0.657708 -1.376027
H -3.126430 0.761116 0.137511
H -1.573507 -0.626120 1.487858
H -1.688051 0.891005 1.759172
H 1.706024 -1.739184 -0.541860
H 2.585593 -1.151259 -1.660827
H 3.535836 1.270502 0.255270
H 3.864200 -0.080936 -0.334023
H 1.528350 -1.650173 1.952638
H 2.888123 -1.642331 1.245917
H -0.434192 1.629426 -0.917817
H -0.231973 0.082437 -0.714699
H 0.282704 2.074681 1.943943
H -0.823350 2.865596 1.215533
H 2.061724 0.387025 1.700748
H 1.355240 1.014696 0.470302
O -1.588431 3.090534 -0.589421
O 2.454561 0.518107 -2.705584
O -3.504878 1.248454 -0.634842
O -2.194286 0.131227 1.412036
O 2.638383 -1.655660 -0.832722
O 4.121085 0.850956 -0.394199
O 2.460245 -1.367552 2.066234
O 0.205572 0.904970 -0.999199
O -0.636924 2.382510 2.031639
O 1.844521 1.243751 1.281403
O -2.386918 -1.295317 -1.614533
O -2.588928 -2.843096 0.089185
C -2.440091 -2.057330 -0.739759
O 0.003620 -1.618331 0.046675
O -0.148719 -1.643828 1.346515

35
i10IV-c: E=-1103.382540900 Ezpc=-1103.105449
H -1.555367 2.495931 -1.261289
H -1.300015 4.035395 -1.487166
H 3.934520 0.268155 0.034616
H 3.228313 1.226209 -0.937442
H -1.615041 0.410472 -1.644378
H -2.782684 0.873971 -0.790930
H -1.926615 -0.096516 0.861051
H -2.485681 1.181949 1.481357
H 1.534442 -1.303581 -1.833971
H 3.020354 -0.915899 -1.727693
H 2.865312 0.211968 2.083514
H 3.106851 -1.171781 1.507356
H 1.092841 -2.028307 0.649161
H 2.292639 -2.398603 -0.202210
H 0.661003 2.490801 -0.982220
H 0.929710 0.980931 -1.128038
H -0.510676 2.201583 2.029984
H -1.215273 3.052628 0.965151
H 0.575544 0.179864 1.519426
H 1.271081 1.390440 0.935734
O -1.015072 3.285687 -0.962069
O 3.895447 0.528111 -0.904825
O -2.299019 1.109689 -1.603958
O -2.766451 0.366421 1.031962
O 2.429471 -1.657857 -1.950483
O 3.578354 -0.353827 1.757964
O 1.985246 -2.406300 0.720996
O 1.348129 1.813963 -0.853834
O -1.340728 2.670278 1.846375
O 1.004213 1.005198 1.791505
O -2.555574 -2.851918 1.047202
O -3.015318 -1.873865 -0.995060
C -2.766897 -2.342345 0.031737
O -0.150359 -0.574617 -1.094533
O -0.413323 -0.939905 0.135953

32
p10-c: E=-914.799606557 Ezpc=-914.535176
H 2.803559 -0.579093 -1.416209
H 3.332052 -1.984529 -1.903501
H -3.085283 -1.462089 -0.183344
H -2.013019 -1.805192 -1.232347
H 1.795345 1.256788 -1.384182
H 3.079933 1.320378 -0.564504
H 1.982804 1.733625 1.132527
H 2.972249 0.639542 1.533430
H -1.723279 1.329752 -1.594311
H -2.853087 0.290558 -1.674814
H -2.175297 -1.260157 1.919981
H -3.037244 -0.068472 1.543836
H -1.649992 1.734826 0.976660
H -2.895101 1.668349 0.110867
H 0.854810 -1.704485 -1.302980
H -0.104911 -0.504603 -1.202028
H 1.745480 -1.311947 1.778512
H 2.770453 -1.524701 0.654456
H -0.166445 -0.113627 1.510604
H -0.215668 -1.408261 0.730276
O 2.714695 -1.571067 -1.298081
O -2.929991 -1.513567 -1.145092
O 2.748556 1.028207 -1.435825
O 2.933548 1.573750 1.264671
O -2.678677 1.246687 -1.739918
O -3.072872 -1.040345 1.634951
O -2.617136 1.656398 1.043039
O -0.070946 -1.472248 -1.115590
O 2.692565 -1.242097 1.577499
O -0.172378 -1.074448 1.645367
O 0.091490 1.334535 -0.825507
O 0.183977 1.543361 0.465369