

Cation Recognition Controlled by Protonation or Chemical Reduction: A Computational Study

Renato Pereira Orenha,^{*a,b} Alexandre Borges,^{c,d} Ana Livia de Oliveira Andrade,^b Sergio Eduardo Ferreira,^b Saulo Samuel Pereira Furtado,^b Vinicius Acir Glitz,^a Giovanni Finoto Caramori,^{*a} and Renato Luis Tame Parreira^{*b}

^a Departamento de Química, Universidade Federal de Santa Catarina, Campus Universitário Trindade, CP 476, Florianópolis, SC, 88040-900, Brazil. E-mail: rpo9@hotmail.com / giovanni.caramori@ufsc.br

^b Núcleo de Pesquisas em Ciências Exatas e Tecnológicas, Universidade de Franca, Franca, SP, Brazil. E-mail: renato.parreira@unifran.edu.br

^c Faculty of Pharmaceutical Sciences, University of Campinas, Campinas, SP, Brazil.

^d Faculdade de Medicina, Centro Universitário de Santa Fé do Sul, Santa Fé do Sul, SP, Brazil.

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QTAIM Analysis

The Recognition of Cations through Deprotonation

The topological analysis of the electron density, carried out by the method QTAIM, revealed bond critical points (BCPs)³³ between the $\mathbf{1}_{\text{OH/O}^-}$ (a-c) receptors and Li^+ , Na^+ or K^+ cations (Figure S5, and Tables S2 and S3). The ratio between the kinetic energy density, G_b , and the potential energy density, V_b , $-G_b/V_b$, at BCPs, correlated with the $\text{C}=\text{O}\cdots\text{Li}^+$, $\text{O}\cdots(\text{Li}^+, \text{Na}^+ \text{ or } \text{K}^+)$, $\text{C}-\text{O}\cdots(\text{Li}^+, \text{Na}^+ \text{ or } \text{K}^+)$, $\text{HN}\cdots\text{Na}^+$ and $\text{ONO}\cdots\text{Na}^+$ bonds show values larger than 1.0, indicating that these interactions are predominantly non-covalent.⁵⁴

In the deprotonation process, the sum of the electron density ($\Delta\rho_b$) at the BCPs: $\text{C}=\text{O}\cdots\text{Li}^+$, $\text{O}\cdots(\text{Li}^+, \text{Na}^+ \text{ or } \text{K}^+)$, $\text{C}-\text{O}\cdots(\text{Li}^+, \text{Na}^+ \text{ or } \text{K}^+)$, $\text{HN}\cdots\text{Na}^+$ and $\text{ONO}\cdots\text{Na}^+$, increase, in agreement with the more attractive ΔE_{oi} energy: i) $\mathbf{1}_{\text{OH(a)}}\cdots\text{Na}^+$ (0.057 a.u. and $-28.39 \text{ kcal mol}^{-1}$) \rightarrow $\mathbf{1}_{\text{O}^-}\text{(a)}\cdots\text{Na}^+$ (0.098 a.u. and $-35.84 \text{ kcal mol}^{-1}$); ii) $\mathbf{1}_{\text{OH(a)}}\cdots\text{K}^+$ (0.083 a.u. and $-26.56 \text{ kcal mol}^{-1}$) \rightarrow $\mathbf{1}_{\text{O}^-}\text{(a)}\cdots\text{K}^+$ (0.099 a.u. and $-30.89 \text{ kcal mol}^{-1}$); and iii) $\mathbf{1}_{\text{OH(c)}}\cdots\text{Na}^+$ (0.070 a.u. and $-34.78 \text{ kcal mol}^{-1}$) \rightarrow $\mathbf{1}_{\text{O}^-}\text{(c)}\cdots\text{Na}^+$ (0.078 a.u. and $-35.80 \text{ kcal mol}^{-1}$). The opposite trend is visualized with the deprotonation of $\mathbf{1}_{\text{OH(b)}}\cdots\text{Na}^+$ (0.079 a.u. and $-36.31 \text{ kcal mol}^{-1}$) to $\mathbf{1}_{\text{O}^-}\text{(b)}\cdots\text{Na}^+$ (0.057 a.u. and $-31.83 \text{ kcal mol}^{-1}$). There are similar values of $\Delta\rho_b$ and ΔE_{oi} in the $\mathbf{1}_{\text{OH(a)}}\cdots\text{Li}^+$ (0.101 a.u. and $-53.28 \text{ kcal mol}^{-1}$) and $\mathbf{1}_{\text{O}^-}\text{(a)}\cdots\text{Li}^+$ (0.100 and $-53.42 \text{ kcal mol}^{-1}$) complexes.

The value of $\Delta\rho_b$ in $\mathbf{1}_{\text{OH(a)}}\cdots\text{K}^+$ (0.083 a.u.) is smaller than in the $\mathbf{1}_{\text{OH(a)}}\cdots\text{Li}^+$ (0.101 a.u.) complex, but larger than in the $\mathbf{1}_{\text{OH(a)}}\cdots\text{Na}^+$ (0.057 a.u.) molecule. The Li^+ cation interacts with: i) four oxygen atoms; and ii) one carbonyl group, of the macrocycle receptor. The Na^+ and K^+ cations interact only with oxygen atoms (five e six O atoms, respectively) of $\mathbf{1}_{\text{OH(a)}}$. This analysis agrees with the more attractive ΔE_{oi} energy in the $\mathbf{1}_{\text{OH(a)}}\cdots\text{Li}^+$ ($-53.28 \text{ kcal mol}^{-1}$) interaction and in the relatively similar ΔE_{oi} energy in the $\mathbf{1}_{\text{OH(a)}}\cdots\text{Na}^+$ ($-28.39 \text{ kcal mol}^{-1}$) and $\mathbf{1}_{\text{OH(a)}}\cdots\text{K}^+$ ($-26.56 \text{ kcal mol}^{-1}$) bonds. There are similar values of $\Delta\rho_b$ (0.098 – 0.100 a.u.) in the $\mathbf{1}_{\text{O}^-}\text{(a)}\cdots(\text{Li}^+, \text{Na}^+ \text{ and } \text{K}^+)$ structures. The more favorable ΔE_{oi} energy in the $\mathbf{1}_{\text{O}^-}\text{(a)}\cdots\text{Li}^+$ ($-53.42 \text{ kcal mol}^{-1}$) interaction concerning the $\mathbf{1}_{\text{O}^-}\text{(a)}\cdots\text{Na}^+$ ($-35.84 \text{ kcal mol}^{-1}$) and $\mathbf{1}_{\text{O}^-}\text{(a)}\cdots\text{K}^+$ ($-30.89 \text{ kcal mol}^{-1}$) bonds, respectively, is elucidated from the increase of ρ_b related to $\text{C}-\text{O}\cdots$ cation BCP: $\mathbf{1}_{\text{O}^-}\text{(a)}\cdots\text{K}^+$ (0.019 a.u.) \rightarrow $\mathbf{1}_{\text{O}^-}\text{(a)}\cdots\text{Na}^+$ (0.027 a.u.) \rightarrow $\mathbf{1}_{\text{O}^-}\text{(a)}\cdots\text{Li}^+$ (0.037 a.u.).

Tuning Carboxylic Acid Functionalized Crown Ethers for Cationic Recognition

The sum of the electron densities at the BCPs between receptor and cation, $\Delta\rho_b$, is larger, in agreement with the more attractive ΔE_{oi} energy, in the $\mathbf{1}_{\text{OH(b)}}\cdots\text{Na}^+$ (0.079 a.u. and $-36.31 \text{ kcal mol}^{-1}$) and $\mathbf{1}_{\text{OH(c)}}\cdots\text{Na}^+$ (0.070 a.u. and $-34.78 \text{ kcal mol}^{-1}$) bonds concerning the $\mathbf{1}_{\text{OH(a)}}\cdots\text{Na}^+$ (0.057 a.u. and $-28.39 \text{ kcal mol}^{-1}$) interaction. On the other hand, there are lower values of $\Delta\rho_b$, which agrees with the less favorable energy ΔE_{oi} , in the $\mathbf{1}_{\text{O}^-}\text{(b)}\cdots\text{Na}^+$ (0.057 a.u. and $-31.83 \text{ kcal mol}^{-1}$) and $\mathbf{1}_{\text{O}^-}\text{(c)}\cdots\text{Na}^+$ (0.078 a.u. and $-35.80 \text{ kcal mol}^{-1}$) interactions than to $\mathbf{1}_{\text{O}^-}\text{(a)}\cdots\text{Na}^+$ (0.098 a.u. and $-35.84 \text{ kcal mol}^{-1}$) bond.

Recognition of Cations by Chemical Reduction

There are BCPs: i) $O\cdots(Li^+, Na^+ \text{ or } K^+)$; ii) $H_2N\cdots Na^+$; iii) $ONO\cdots Na^+$ (Figures S11 and S12), between the $2_{Fe^+/Fe}(a-e)$ receptors and Li^+ , Na^+ or K^+ cations with $-G_b/V_b$ values larger than 1.0 (Tables S4 and S5), indicating that these interactions are predominantly non-covalent.⁵⁴ The sum of the electron density at these BCPs, $\Delta\rho_b$, increase after the chemical reduction process in the $2_{Fe^+}(a)\cdots Li^+$ (0.093 \rightarrow 0.101 a.u.) and $2_{Fe^+}(a)\cdots K^+$ (0.070 \rightarrow 0.089 a.u.) compounds, in agreement with the similar or more attractive ΔE_{oi} energy in the $2_{Fe}(a)\cdots Li^+$ ($-52.96 \text{ kcal mol}^{-1}$) and $2_{Fe}(a)\cdots K^+$ ($-29.76 \text{ kcal mol}^{-1}$) bonds regarding the $2_{Fe^+}(a)\cdots Li^+$ ($-52.44 \text{ kcal mol}^{-1}$) and $2_{Fe^+}(a)\cdots K^+$ ($-26.42 \text{ kcal mol}^{-1}$) interactions, respectively. The chemical reduction of $2_{Fe^+}(a)\cdots Na^+$ leading to $2_{Fe}(a)\cdots Na^+$ decrease the value of $\Delta\rho_b$ (0.076 \rightarrow 0.073 a.u.) in agreement with the less attractive ΔE_{oi} energy of $2_{Fe}(a)\cdots Na^+$ ($-30.93 \text{ kcal mol}^{-1}$) in relation to $2_{Fe^+}(a)\cdots Na^+$ ($-33.03 \text{ kcal mol}^{-1}$).

The reduction of the $2_{Fe^+}(b)\cdots Na^+$ complex decrease the $\Delta\rho_b$ value (0.087 \rightarrow 0.080 a.u.), which is not consistent with the more favorable ΔE_{oi} energy in the $2_{Fe}(b)\cdots Na^+$ structure ($-37.25 \text{ kcal mol}^{-1}$) compared to $2_{Fe^+}(b)\cdots Na^+$ compound ($-35.74 \text{ kcal mol}^{-1}$). It can be explained considering the larger number of interactions $H_2N\cdots Na^+$ in the $2_{Fe}(b)\cdots Na^+$ complex (2x) regarding the $2_{Fe^+}(b)\cdots Na^+$ molecule (1x). The reduction of the $2_{Fe^+}(c)\cdots Na^+$ compound increase the $\Delta\rho_b$ value (0.074 \rightarrow 0.085 a.u.), which does not agree with the less attractive ΔE_{oi} energy in the $2_{Fe}(c)\cdots Na^+$ complex ($-36.03 \text{ kcal mol}^{-1}$) concerning $2_{Fe^+}(c)\cdots Na^+$ ($-39.02 \text{ kcal mol}^{-1}$). This can be explained by the decrease in number of $ONO\cdots Na^+$ BCPs in the $2_{Fe^+}(c)\cdots Na^+$ compound (2x) in relation to $2_{Fe}(c)\cdots Na^+$ molecule (1x). There are similar $\Delta\rho_b$ and ΔE_{oi} values in the $2_{Fe}(d)\cdots Na^+$ (0.083 a.u. and $-36.91 \text{ kcal mol}^{-1}$) and $2_{Fe^+}(d)\cdots Na^+$ (0.080 a.u. and $-36.30 \text{ kcal mol}^{-1}$) molecules. The $\Delta\rho_b$ value increase after the chemical reduction process in the $2_{Fe^+}(e)\cdots Na^+$ molecule (0.063 \rightarrow 0.077 a.u.), which agrees with the more favorable ΔE_{oi} energy in the $2_{Fe}(e)\cdots Na^+$ interaction ($-37.46 \text{ kcal mol}^{-1}$) compared to $2_{Fe^+}(e)\cdots Na^+$ bond ($-34.44 \text{ kcal mol}^{-1}$).

The increase of the cation size in the $2_{Fe^+}(a)\cdots(Li^+, Na^+ \text{ or } K^+)$ interactions is followed by decrease of the values of $\Delta\rho_b$ (0.093 \rightarrow 0.076 \rightarrow 0.070 a.u.) in agreement with a respectively less attractive ΔE_{oi} energy ($-52.44 \rightarrow -33.03 \rightarrow -26.42 \text{ kcal mol}^{-1}$). The increase of the cation size in the $2_{Fe}(a)\cdots(Li^+ \text{ or } Na^+)$ bonds is followed by decrease of the values of $\Delta\rho_b$ (0.101 \rightarrow 0.073 a.u.), which is in agreement with a respectively less attractive ΔE_{oi} energy ($-52.96 \rightarrow -30.93 \text{ kcal mol}^{-1}$). However, the increase of the cation size in the $2_{Fe}(a)\cdots(Na^+ \text{ or } K^+)$ interactions is not followed by a decrease of the values of $\Delta\rho_b$ (0.073 \rightarrow 0.089 a.u.) and, therefore, does not agree with a slightly less attractive ΔE_{oi} energy ($-30.93 \rightarrow -29.76 \text{ kcal mol}^{-1}$). It can be explained by the more favorable ΔE_{disp} energy in the $2_{Fe}(a)\cdots K^+$ bond ($-13.65 \text{ kcal mol}^{-1}$) concerning the $2_{Fe}(a)\cdots Na^+$ interaction ($-12.11 \text{ kcal mol}^{-1}$).

Tuning Ferrocenes Functionalized Crown Ethers to Cationic Recognition

The QTAIM method shows that, on the whole, there are larger $\Delta\rho_b$ values at the BCPs present between the $2_{Fe^+/Fe}(b-e)$ receptors and Na^+ cation, in agreement with the more negative ΔE_{oi} values, compared to $2_{Fe^+/Fe}(a)\cdots Na^+$ interactions (Tables 1, S1, S4 and S5).

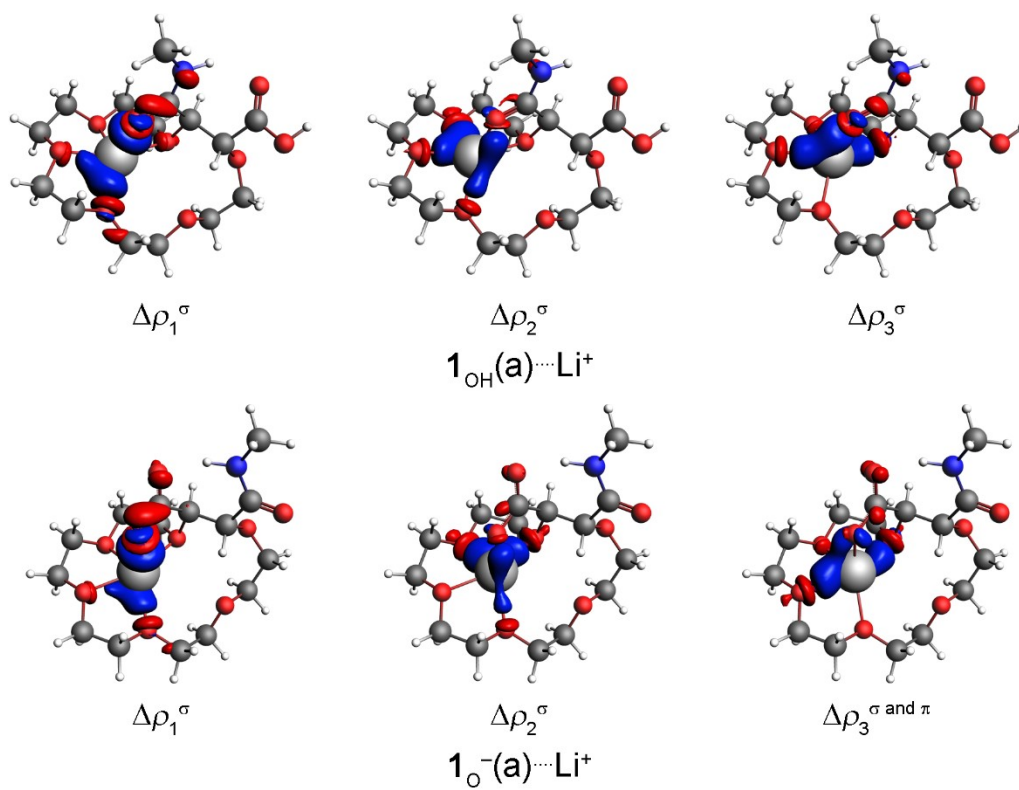


Figure S1. The surface of the main density deformation channels with isovalue = 0.001 a.u., where the red and blue regions indicate the electronic density outflow and inflow, to $\mathbf{1}_{\text{OH/O}^-}(\text{a})\cdots\text{Li}^+$ complexes, respectively. Atoms color code: H = white; C = gray; N = blue; O = red; and Li = light gray.

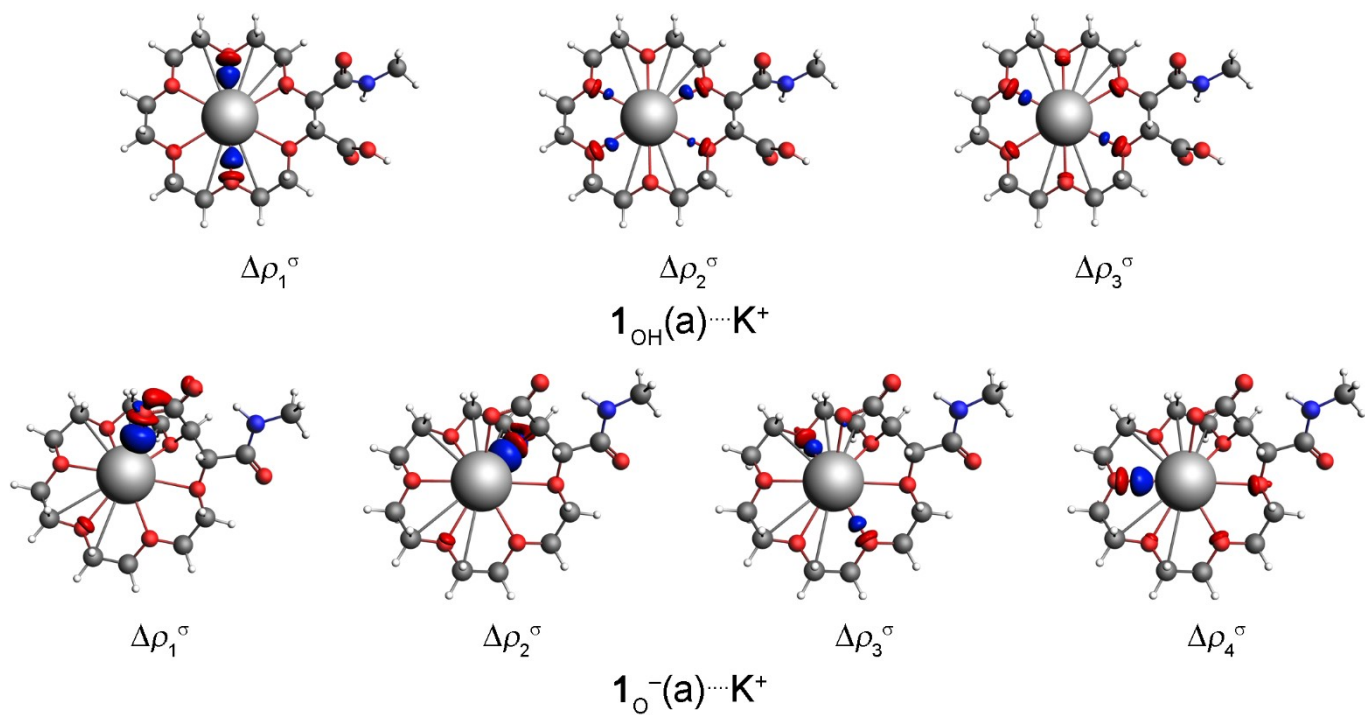


Figure S2. The surface of the main density deformation channels with isovalue = 0.001 a.u., where the red and blue regions indicate the electronic density outflow and inflow, to $\mathbf{1}_{\text{OH/O}^-}(\mathbf{a})\cdots\text{K}^+$ complexes, respectively. Atoms color code: H = white; C = gray; N = blue; O = red; and K = light gray.

Table S1. Analysis of the bonding situation between the receptors class: **1**_{OH/O⁻} or **2**_{Fe⁺/Fe⁻}, and cation (Na⁺) through of the EDA–NOCV method. The unit of energy is kcal mol⁻¹.^[a,b]

Complex	ΔE	ΔE_{prep}	ΔE_{int}	ΔV_{elstat}	ΔE_{Pauli}	ΔE_{oi}	ΔE_{disp}	$\Delta E_{\text{oi},1}$	$\Delta E_{\text{oi},2}$	$\Delta E_{\text{oi},3}$	$\Delta E_{\text{oi},4}$	$\Delta E_{\text{oi},5}$	$\Delta E_{\text{oi},6}$	$q_{\text{VDD}}^{\text{Cation}}$
1 _{OH(b)} ⋯Na ⁺	-82.88	22.01	-104.89	-80.16 (62)	24.85	-36.31 (28)	-13.27 (10)	-4.41	-3.10	-2.98	-2.66	-2.25	-	-0.084
1 _{O⁻(b)} ⋯Na ⁺	-140.01	19.93	-159.94	-130.70 (75)	15.08	-31.83 (18)	-12.50 (7)	-3.94	-2.58	-2.53	-2.03	-	-	-0.078
1 _{OH(c)} ⋯Na ⁺	-59.57	6.12	-65.69	-38.18 (47)	15.84	-34.78 (43)	-8.56 (11)	-3.89	-3.03	-2.70	-2.45	-	-	-0.066
1 _{O⁻(c)} ⋯Na ⁺	-112.58	2.80	-115.38	-87.34 (66)	17.41	-35.80 (27)	-9.65 (7)	-3.79	-2.96	-2.23	-2.19	-2.27	-2.14	-0.069
2 _{Fe⁺(b)} ⋯Na ⁺	-23.25	26.28	-49.53	-25.98 (35)	24.48	-35.74 (48)	-12.29 (17)	-6.26	-	-	-	-	-	-0.085
2 _{Fe(b)} ⋯Na ⁺	-97.21	15.28	-112.49	-83.44 (62)	21.66	-37.25 (28)	-13.45 (10)	-4.51	-3.22	-2.71	-2.67	-2.43	-	-0.100
2 _{Fe⁺(c)} ⋯Na ⁺	13.12	13.04	0.08	28.71 (-) ^[c]	21.56	-39.02 (78) ^[c]	-11.17 (22) ^[c]	-6.70	-4.06	-2.41	-3.34	-	-	-0.080
2 _{Fe(c)} ⋯Na ⁺	-58.84	8.27	-67.11	-44.64 (49)	24.10	-36.03 (40)	-10.54 (12)	-2.87	-3.96	-3.03	-2.71	-	-	-0.074
2 _{Fe⁺(d)} ⋯Na ⁺	-20.80	20.47	-41.27	-15.11 (24)	22.42	-36.30 (57)	-12.28 (19)	-6.21	-4.32	-	-	-	-	-0.091
2 _{Fe(d)} ⋯Na ⁺	-24.57	73.13	-97.70	-71.34 (59)	24.09	-36.91 (30)	-13.55 (11)	-4.27	-3.11	-2.97	-	-	-	-0.095
2 _{Fe⁺(e)} ⋯Na ⁺	8.97	15.38	-6.41	20.63 (-) ^[c]	15.77	-34.44 (80) ^[c]	-8.37 (20) ^[c]	-3.72	-4.41	-3.20	-3.09	-2.45	-	-0.066
2 _{Fe(e)} ⋯Na ⁺	-54.81	8.11	-62.92	-35.88 (42)	22.36	-37.46 (44)	-11.94 (14)	-3.75	-2.87	-2.43	-2.65	-2.17	-2.06	-0.076

^[a] $\Delta E_{\text{int}} = \Delta V_{\text{elstat}} + \Delta E_{\text{Pauli}} + \Delta E_{\text{oi}} + \Delta E_{\text{disp}}$; ^[b] Values in parentheses correspond to the percentage of each stabilizing contribution ($\Delta V_{\text{elstat}} + \Delta E_{\text{oi}} + \Delta E_{\text{disp}} = 100\%$). ^[c] Values in parentheses correspond to the percentage of each stabilizing contribution ($\Delta E_{\text{oi}} + \Delta E_{\text{disp}} = 100\%$) since that ΔV_{elstat} have a repulsive contribution.

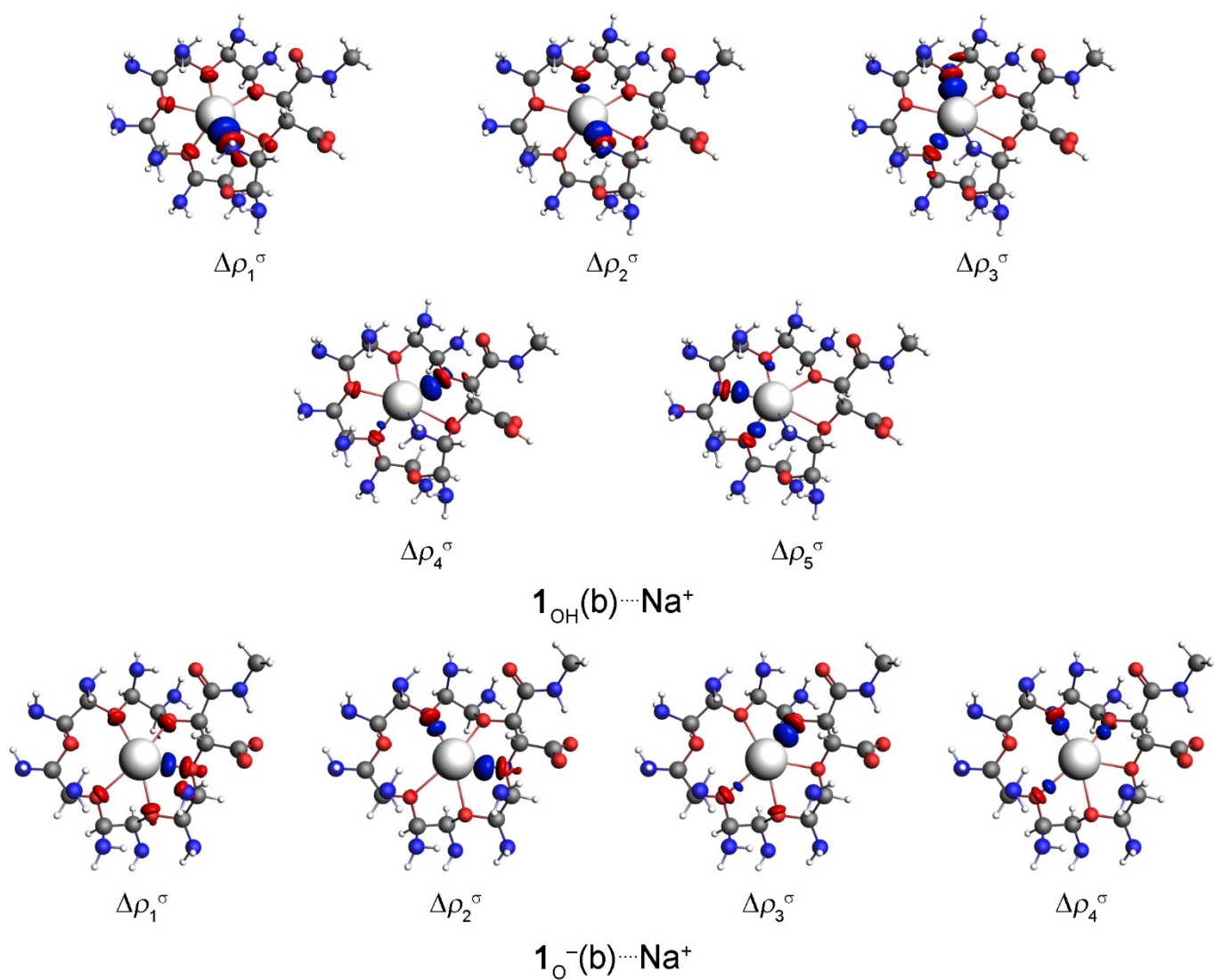


Figure S3. The surface of the main density deformation channels with isovalue = 0.001 a.u., where the red and blue regions indicate the electronic density outflow and inflow, to $\mathbf{1}_{\text{OH/O}^-}(\text{b})\cdots\text{Na}^+$ complexes, respectively. Atoms color code: H = white; C = gray; N = blue; O = red; and Na = ice.

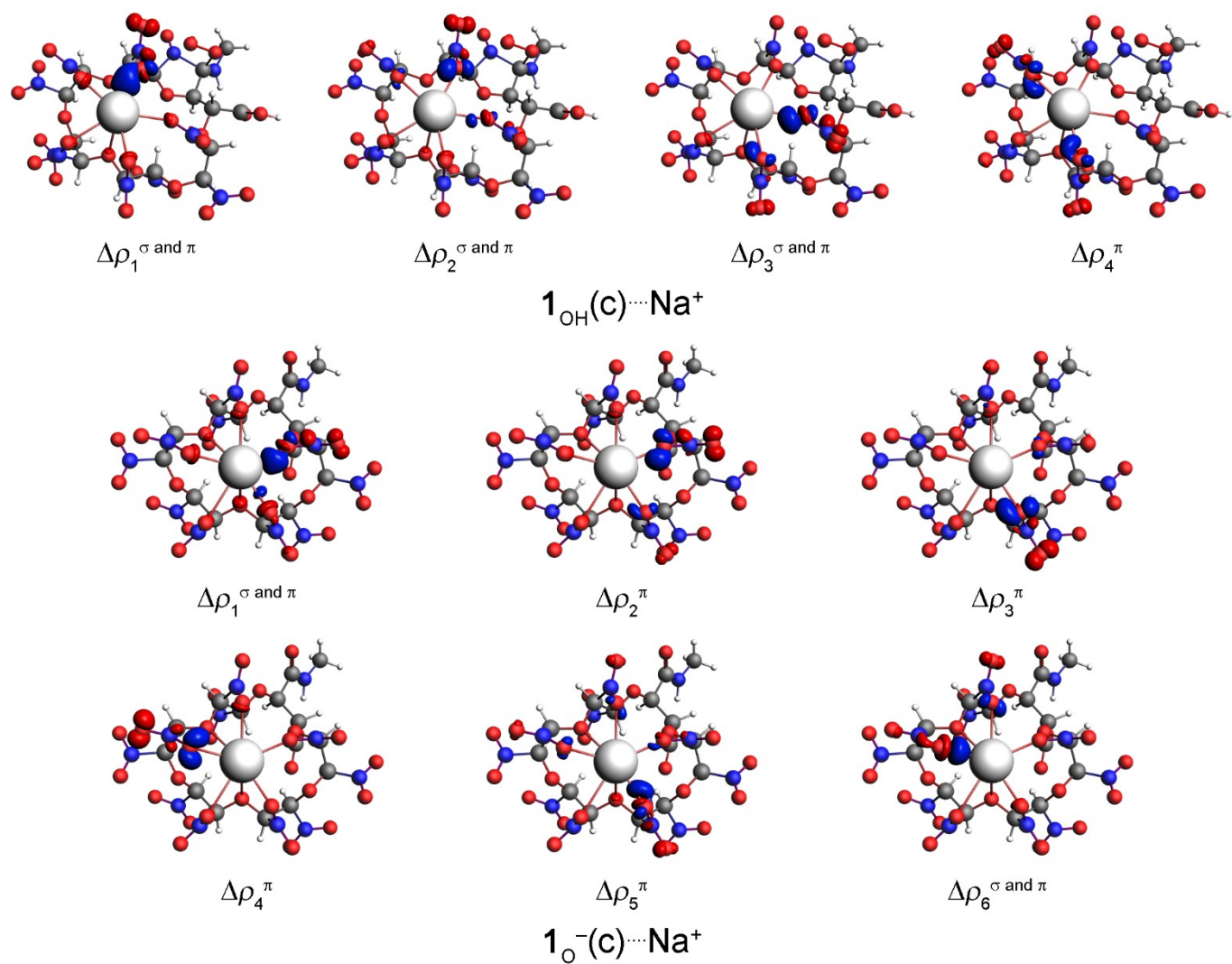


Figure S4. The surface of the main density deformation channels with isovalue = 0.001 a.u., where the red and blue regions indicate the electronic density outflow and inflow, to $\mathbf{1}_{\text{OH/O}^-(\text{c})\cdots\text{Na}^+}$ complexes, respectively. Atoms color code: H = white; C = gray; N = blue; O = red; and Na = ice.

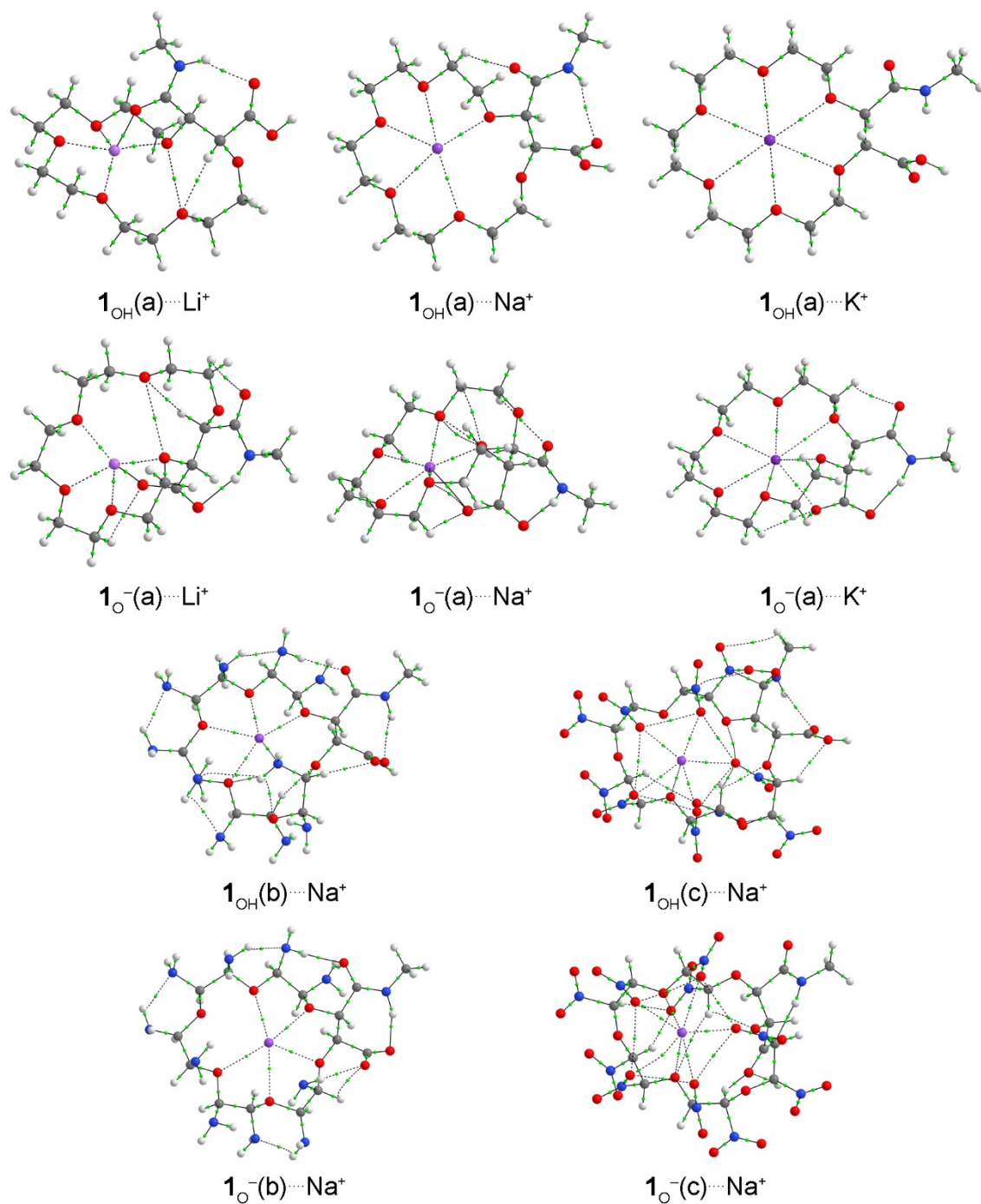


Figure S5. Topological map showing the bond paths (continuous or dashed lines connecting the attractors) and bond critical points (small green points), for the $1_{\text{OH/O}}(\text{a-c}) \cdots (\text{Li}^+, \text{Na}^+ \text{ or } \text{K}^+)$ complexes. Atoms color code: H = white; C = gray; N = blue; O = red; Li = light purple; Na = purple; and K = dark purple.

Table S2. Ratio between the kinetic energy density, G_b , and potential energy density, V_b , $-G_b/V_b$, and electron density, ρ_b , at BCPs related to interactions between the $\mathbf{1}_{\text{OH/O}^-}(\text{a})$ receptors and cations (Li^+ , Na^+ or K^+). The values of all the parameters are given in a.u.

Complex	BCP	$-G_b/V_b$	ρ_b
$\mathbf{1}_{\text{OH}(\text{a})}\cdots\text{Li}^+$	$\text{C}=\text{O}\cdots\text{Li}^+$	1.219	0.030
	$\text{O}\cdots\text{Li}^+$	1.300	0.018
	$\text{O}\cdots\text{Li}^+$	1.308	0.014
	$\text{O}\cdots\text{Li}^+$	1.284	0.020
	$\text{O}\cdots\text{Li}^+$	1.293	0.020
$\mathbf{1}_{\text{O}^-}(\text{a})\cdots\text{Li}^+$	$\text{C}-\text{O}\cdots\text{Li}^+$	1.172	0.037
	$\text{O}\cdots\text{Li}^+$	1.344	0.015
	$\text{O}\cdots\text{Li}^+$	1.276	0.018
	$\text{O}\cdots\text{Li}^+$	1.331	0.015
	$\text{O}\cdots\text{Li}^+$	1.329	0.016
$\mathbf{1}_{\text{OH}(\text{a})}\cdots\text{Na}^+$	$\text{O}\cdots\text{Na}^+$	1.416	0.012
	$\text{O}\cdots\text{Na}^+$	1.420	0.013
	$\text{O}\cdots\text{Na}^+$	1.435	0.011
	$\text{O}\cdots\text{Na}^+$	1.421	0.012
	$\text{O}\cdots\text{Na}^+$	1.471	0.008
$\mathbf{1}_{\text{O}^-}(\text{a})\cdots\text{Na}^+$	$\text{C}-\text{O}\cdots\text{Na}^+$	1.237	0.027
	$\text{O}\cdots\text{Na}^+$	1.437	0.011
	$\text{O}\cdots\text{Na}^+$	1.381	0.014
	$\text{O}\cdots\text{Na}^+$	1.387	0.015
	$\text{O}\cdots\text{Na}^+$	1.329	0.019
	$\text{O}\cdots\text{Na}^+$	1.414	0.012
$\mathbf{1}_{\text{OH}(\text{a})}\cdots\text{K}^+$	$\text{O}\cdots\text{K}^+$	1.300	0.015
	$\text{O}\cdots\text{K}^+$	1.315	0.014
	$\text{O}\cdots\text{K}^+$	1.329	0.013
	$\text{O}\cdots\text{K}^+$	1.329	0.013
	$\text{O}\cdots\text{K}^+$	1.306	0.015
	$\text{O}\cdots\text{K}^+$	1.353	0.012
$\mathbf{1}_{\text{O}^-}(\text{a})\cdots\text{K}^+$	$\text{C}-\text{O}\cdots\text{K}^+$	1.226	0.019
	$\text{O}\cdots\text{K}^+$	1.343	0.013
	$\text{O}\cdots\text{K}^+$	1.422	0.009
	$\text{O}\cdots\text{K}^+$	1.222	0.020
	$\text{O}\cdots\text{K}^+$	1.341	0.013
	$\text{O}\cdots\text{K}^+$	1.314	0.014
	$\text{O}\cdots\text{K}^+$	1.385	0.011

Table S3. Ratio between the kinetic energy density, G_b , and the potential energy density, V_b , $-G_b/V_b$, and the electron density, ρ_b , at BCPs related to interactions between the $\mathbf{1}_{\text{OH/O}^-}$ (b or c) receptors and the cation (Na^+). The values of all the parameters are given in a.u.

Complex	BCP	$-G_b/V_b$	ρ_b
$\mathbf{1}_{\text{OH}(b)}\cdots\text{Na}^+$	O $\cdots\text{Na}^+$	1.298	0.022
	O $\cdots\text{Na}^+$	1.393	0.014
	O $\cdots\text{Na}^+$	1.413	0.012
	O $\cdots\text{Na}^+$	1.367	0.016
	HN $\cdots\text{Na}^+$	1.305	0.015
$\mathbf{1}_{\text{O}^-(b)}\cdots\text{Na}^+$	O $\cdots\text{Na}^+$	1.461	0.009
	O $\cdots\text{Na}^+$	1.394	0.014
	O $\cdots\text{Na}^+$	1.462	0.009
	O $\cdots\text{Na}^+$	1.358	0.016
	O $\cdots\text{Na}^+$	1.436	0.010
$\mathbf{1}_{\text{OH}(c)}\cdots\text{Na}^+$	ONO $\cdots\text{Na}^+$	1.412	0.015
	ONO $\cdots\text{Na}^+$	1.433	0.014
	ONO $\cdots\text{Na}^+$	1.491	0.008
	ONO $\cdots\text{Na}^+$	1.411	0.014
	ONO $\cdots\text{Na}^+$	1.474	0.011
	O $\cdots\text{Na}^+$	1.461	0.008
$\mathbf{1}_{\text{O}^-(c)}\cdots\text{Na}^+$	ONO $\cdots\text{Na}^+$	1.462	0.011
	ONO $\cdots\text{Na}^+$	1.417	0.014
	ONO $\cdots\text{Na}^+$	1.408	0.005
	ONO $\cdots\text{Na}^+$	1.389	0.016
	ONO $\cdots\text{Na}^+$	1.410	0.016
	O $\cdots\text{Na}^+$	1.426	0.007
	O $\cdots\text{Na}^+$	1.464	0.008

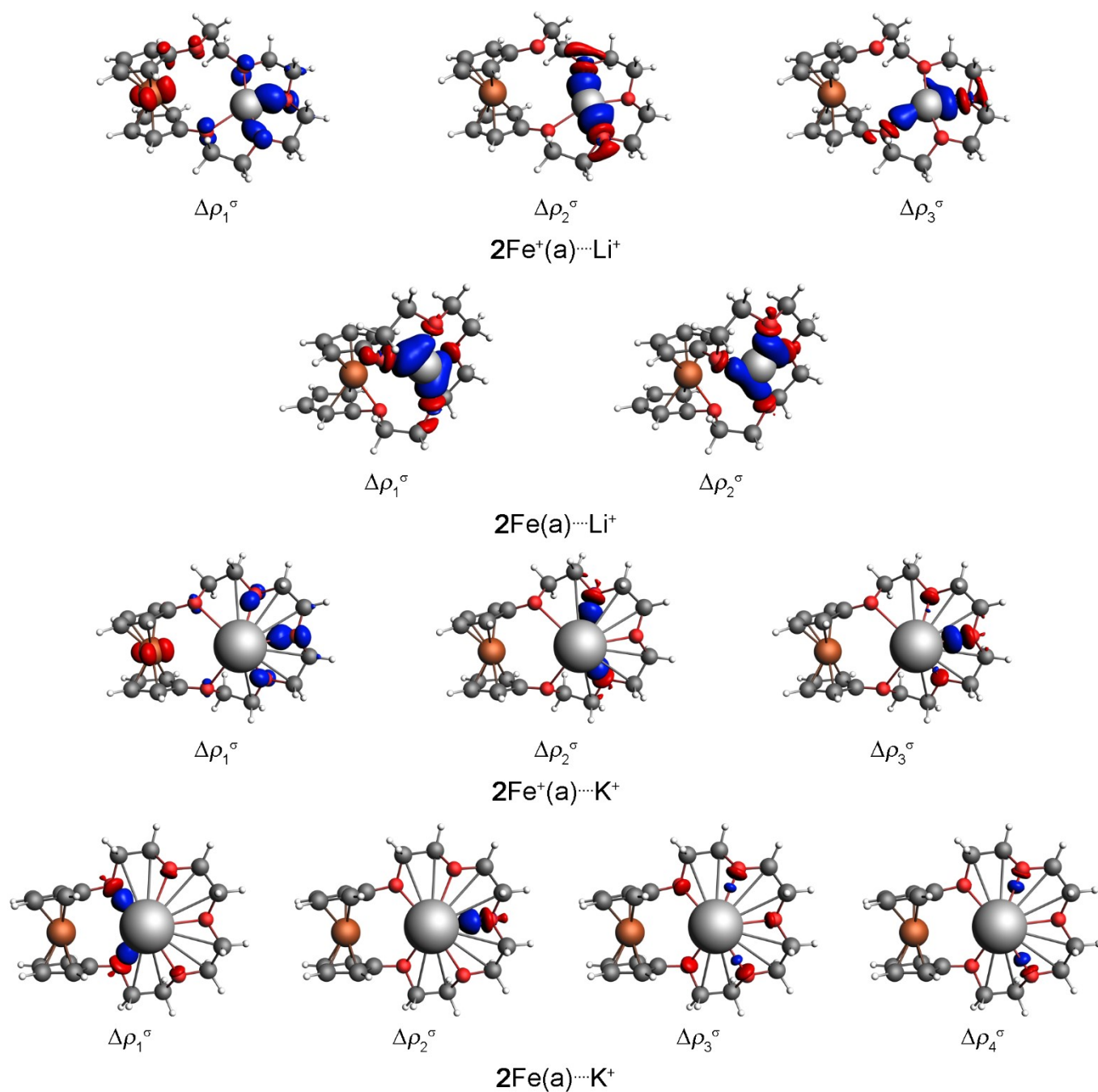


Figure S6. The main density deformation channel surface plots with isovalue = 0.001 a.u., where the red and blue regions indicate the electronic density outflow and inflow, respectively, to $2\text{Fe}^+_{/\text{Fe}}(\text{a})\cdots(\text{Li}^+ \text{ or } \text{K}^+)$ complexes. Atoms color code: H = white; C = gray; O = red; Li = light gray; K = light gray; and Fe = brown.

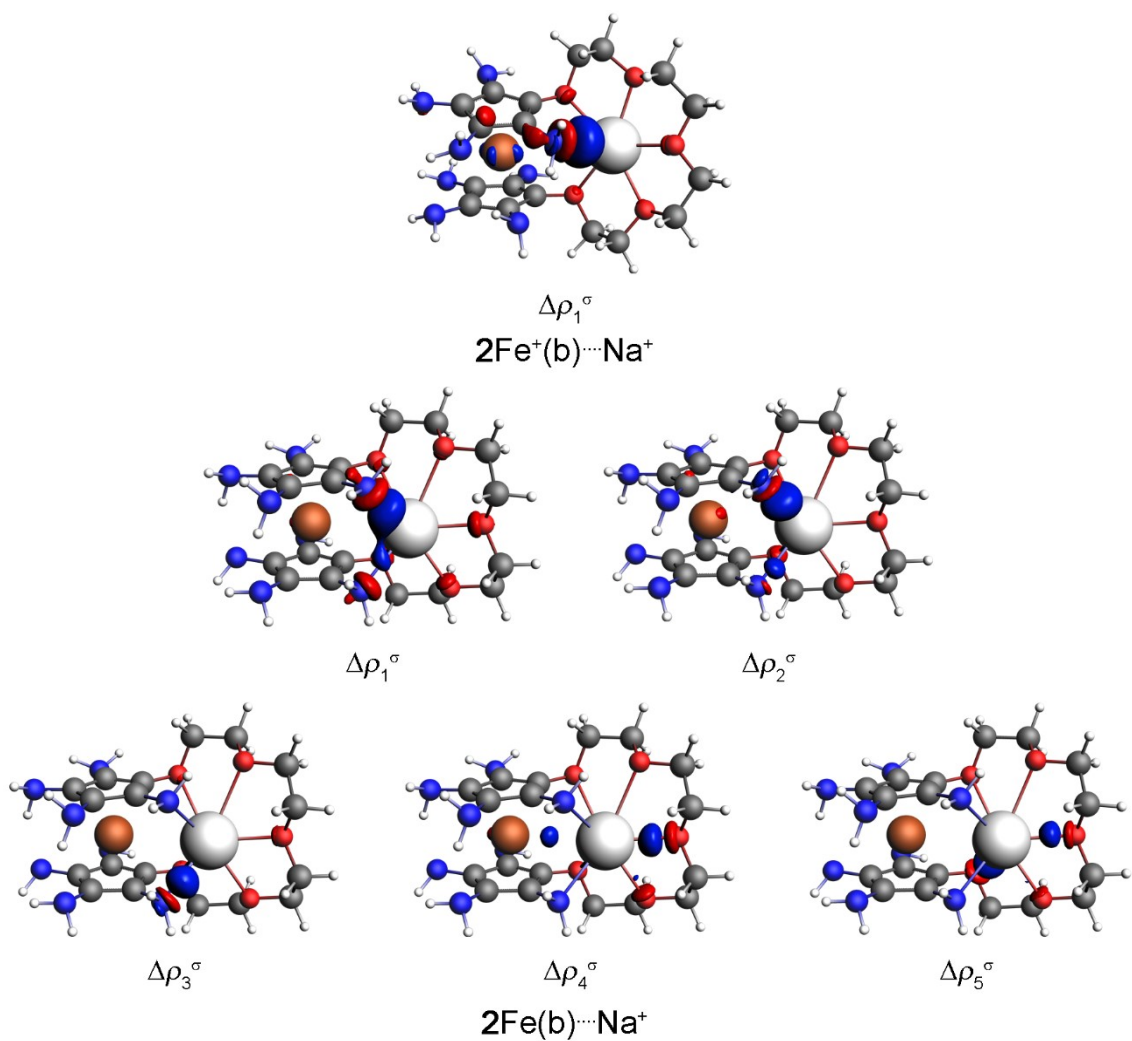


Figure S7. The surface of the main density deformation channels with isovalue = 0.001 a.u., where the red and blue regions indicate the electronic density outflow and inflow, to $2\text{Fe}^+/\text{Fe}(\text{b})\cdots\text{Na}^+$ complexes, respectively,. Atoms color code: H = white; C = gray; N = blue; O = red; Na = ice; and Fe = brown.

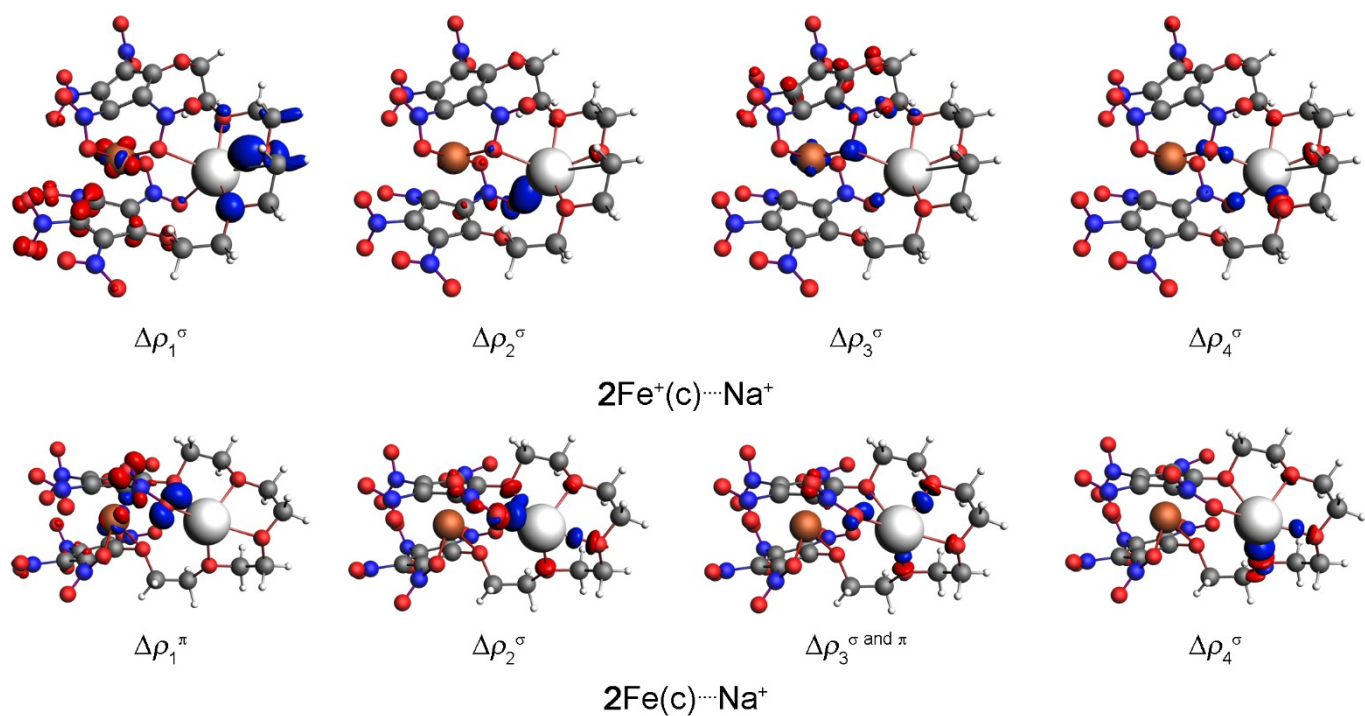


Figure S8. The surface of the main density deformation channels with isovalue = 0.001 a.u., where the red and blue regions indicate the electronic density outflow and inflow, to $2\text{Fe}^+_{/\text{Fe}}(\text{c})\cdots\text{Na}^+$ complexes, respectively. Atoms color code: H = white; C = gray; N = blue; O = red; Na = ice; and Fe = brown.

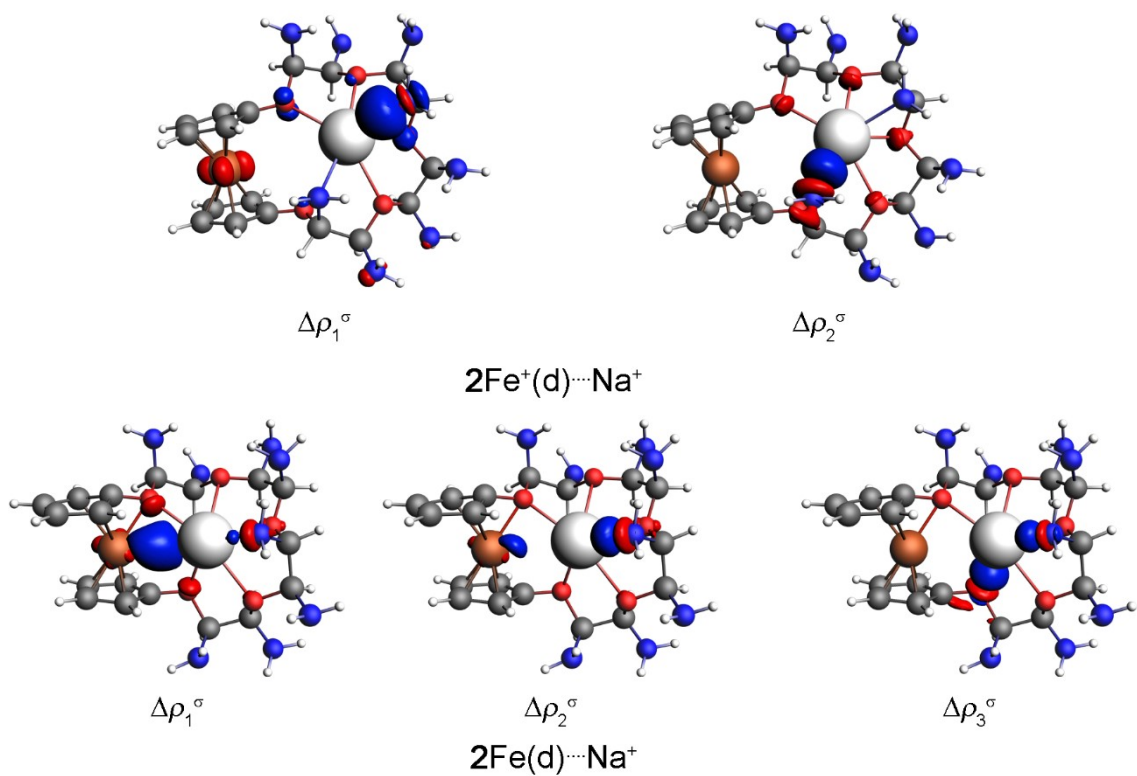


Figure S9. The surface of the main density deformation channels with isovalue = 0.001 a.u., where the red and blue regions indicate the electronic density outflow and inflow, to $2\text{Fe}^+_{/\text{Fe}(\text{d})}\cdots\text{Na}^+$ complexes, respectively. Atoms color code: H = white; C = gray; N = blue; O = red; Na = ice; and Fe = brown.

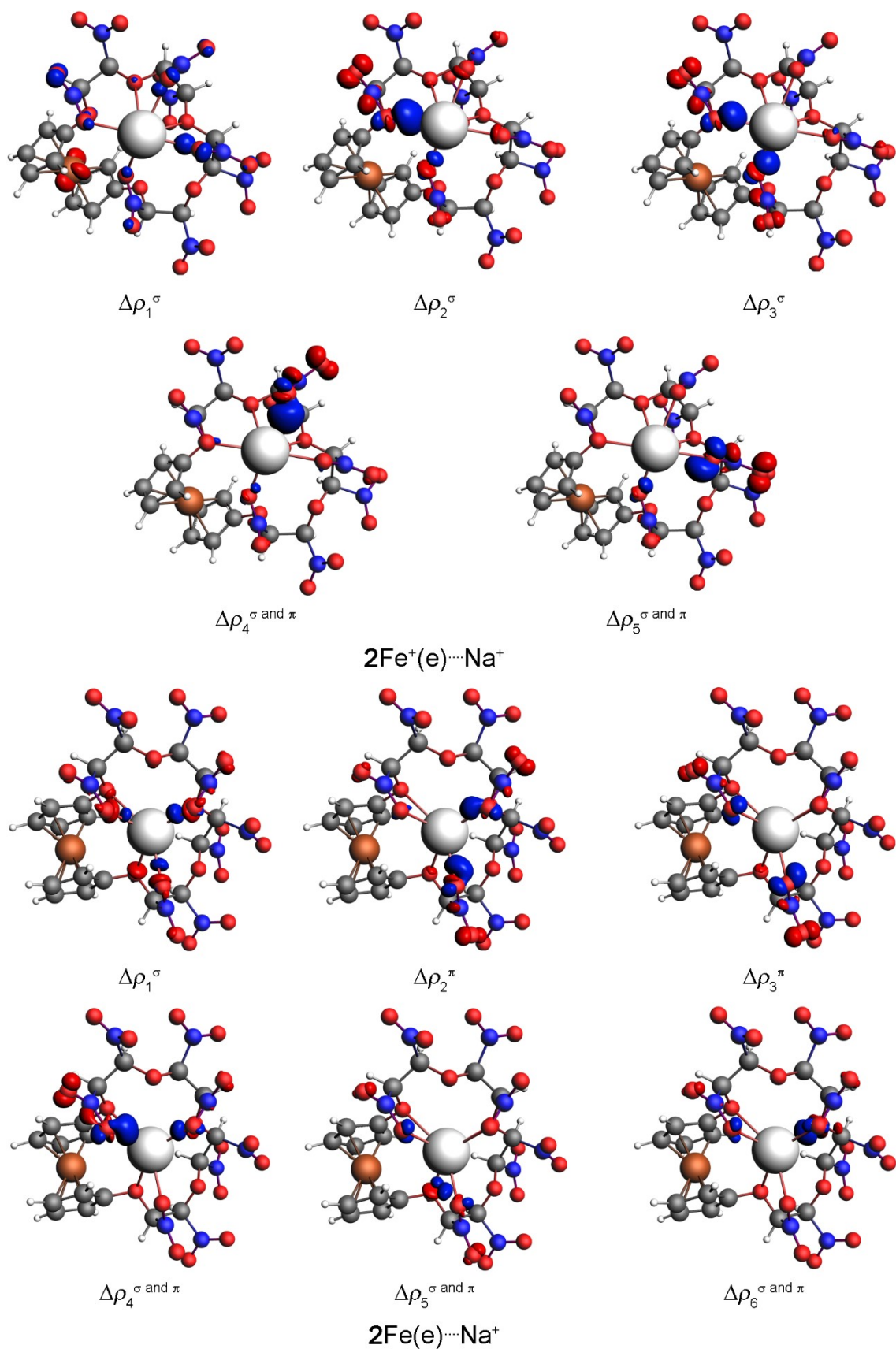


Figure S10. The surface of the main density deformation channels with isovalue = 0.001 a.u., where the red and blue regions indicate the electronic density outflow and inflow, to $2\text{Fe}^+_{/\text{Fe}}(\text{e})\cdots\text{Na}^+$ complexes, respectively. Atoms color code: H = white; C = gray; N = blue; O = red; Na = ice; and Fe = brown.

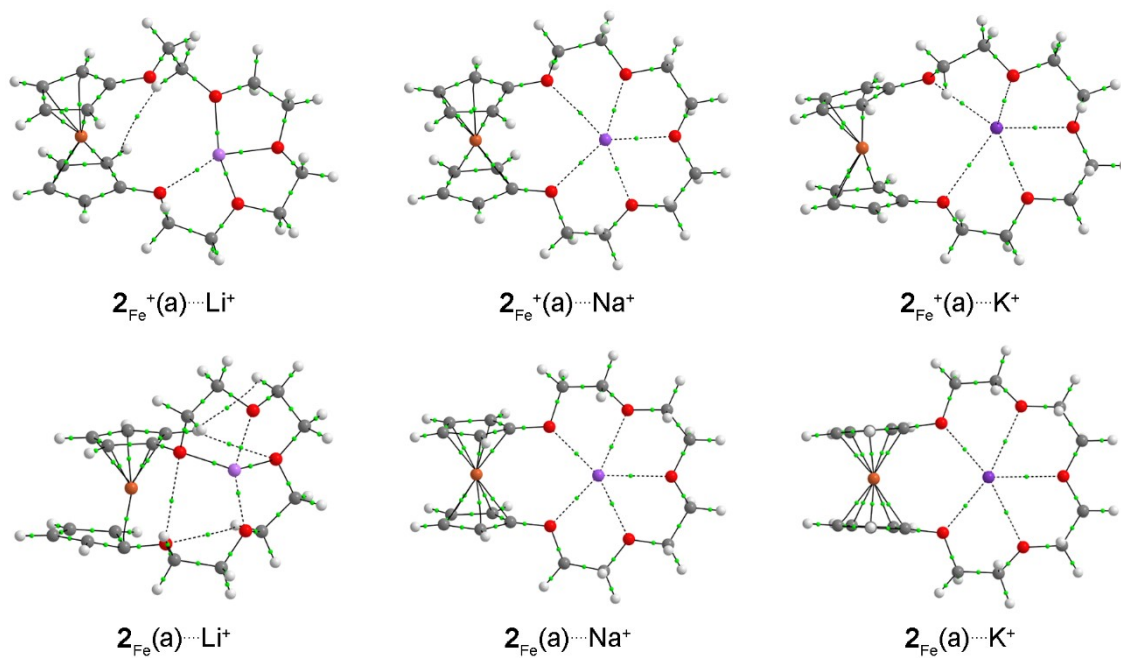


Figure S11. Topological map showing the bond paths (continuous or dashed lines connecting the attractors) and bond critical points (small green points), for the $2_{\text{Fe}^+/\text{Fe}}(\text{a})\cdots(\text{Li}^+, \text{Na}^+ \text{ or } \text{K}^+)$ complexes. Atoms color code: H = white; C = gray; O = red; Li = light purple; Na = purple; K = dark purple; and Fe = brown.

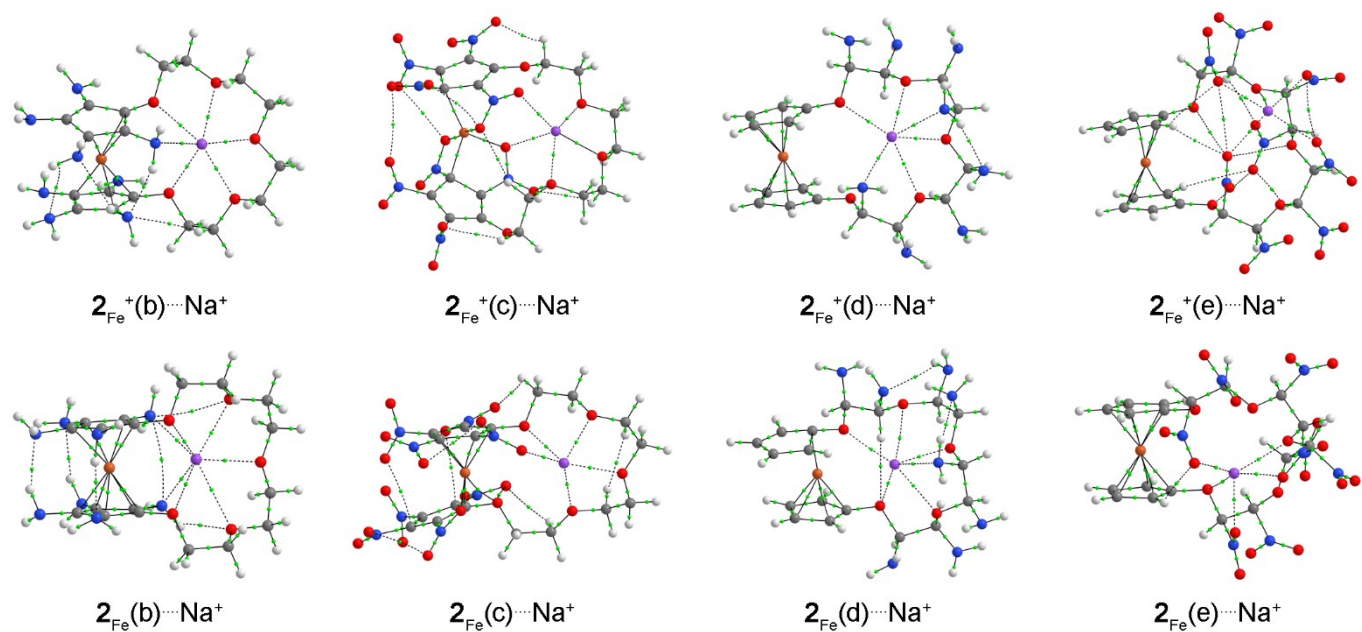


Figure S12. Topological map showing the bond paths (continuous or dashed lines connecting the attractors) and bond critical points (small green points), for the $2_{\text{Fe}^+/\text{Fe}^-}(\text{b-e})\cdots\text{Na}^+$ complexes. Atoms color code: H = white; C = gray; N = blue; O = red; Na = purple; and Fe = brown.

Table S4. Ratio between the kinetic energy density, G_b , and the potential energy density, V_b , $-G_b/V_b$, and the electron density, ρ_b , at BCPs related to interactions between the $2_{Fe}^+/_{Fe}(a)$ receptors and the cations (Li^+ , Na^+ or K^+). The values of all the parameters are given in a.u.

Complex	BCP	$-G_b/V_b$	ρ_b
$2_{Fe}^+(a)\cdots Li^+$	O \cdots Li $^+$	1.389	0.011
	O \cdots Li $^+$	1.212	0.028
	O \cdots Li $^+$	1.230	0.026
	O \cdots Li $^+$	1.211	0.028
$2_{Fe}(a)\cdots Li^+$	O \cdots Li $^+$	1.223	0.026
	O \cdots Li $^+$	1.241	0.022
	O \cdots Li $^+$	1.236	0.025
	O \cdots Li $^+$	1.211	0.027
$2_{Fe}^+(a)\cdots Na^+$	O \cdots Na $^+$	1.475	0.006
	O \cdots Na $^+$	1.425	0.012
	O \cdots Na $^+$	1.329	0.019
	O \cdots Na $^+$	1.319	0.019
	O \cdots Na $^+$	1.313	0.020
$2_{Fe}(a)\cdots Na^+$	O \cdots Na $^+$	1.375	0.016
	O \cdots Na $^+$	1.375	0.016
	O \cdots Na $^+$	1.392	0.014
	O \cdots Na $^+$	1.407	0.013
	O \cdots Na $^+$	1.391	0.014
$2_{Fe}^+(a)\cdots K^+$	O \cdots K $^+$	1.466	0.008
	O \cdots K $^+$	1.482	0.008
	O \cdots K $^+$	1.248	0.018
	O \cdots K $^+$	1.250	0.018
	O \cdots K $^+$	1.265	0.017
$2_{Fe}(a)\cdots K^+$	O \cdots K $^+$	1.220	0.020
	O \cdots K $^+$	1.221	0.020
	O \cdots K $^+$	1.286	0.016
	O \cdots K $^+$	1.270	0.017
	O \cdots K $^+$	1.283	0.016

Table S5. Ratio between the kinetic energy density, G_b , and the potential energy density, V_b , $-G_b/V_b$, and the electron density, ρ_b , at BCPs related to interactions between the $2_{Fe^+}/Fe(b-e)$ receptors and the cation (Na^+). The values of all the parameters are given in a.u.

Complex	BCP	$-G_b/V_b$	ρ_b
$2_{Fe^+}(b)\cdots Na^+$	O $\cdots Na^+$	1.360	0.017
	O $\cdots Na^+$	1.431	0.012
	O $\cdots Na^+$	1.375	0.015
	O $\cdots Na^+$	1.377	0.015
	O $\cdots Na^+$	1.436	0.011
	H ₂ N $\cdots Na^+$	1.291	0.017
$2_{Fe}(b)\cdots Na^+$	O $\cdots Na^+$	1.383	0.015
	O $\cdots Na^+$	1.386	0.015
	O $\cdots Na^+$	1.430	0.011
	O $\cdots Na^+$	1.422	0.005
	O $\cdots Na^+$	1.464	0.007
	H ₂ N $\cdots Na^+$	1.312	0.015
	H ₂ N $\cdots Na^+$	1.345	0.012
$2_{Fe^+}(c)\cdots Na^+$	O $\cdots Na^+$	1.411	0.013
	O $\cdots Na^+$	1.367	0.016
	O $\cdots Na^+$	1.251	0.026
	ONO $\cdots Na^+$	1.488	0.008
	ONO $\cdots Na^+$	1.456	0.011
$2_{Fe}(c)\cdots Na^+$	O $\cdots Na^+$	1.369	0.016
	O $\cdots Na^+$	1.403	0.014
	O $\cdots Na^+$	1.358	0.017
	O $\cdots Na^+$	1.323	0.019
	ONO $\cdots Na^+$	1.364	0.018
$2_{Fe^+}(d)\cdots Na^+$	O $\cdots Na^+$	1.430	0.009
	O $\cdots Na^+$	1.464	0.010
	O $\cdots Na^+$	1.338	0.018
	O $\cdots Na^+$	1.370	0.015
	H ₂ N $\cdots Na^+$	1.326	0.013
	H ₂ N $\cdots Na^+$	1.309	0.015
$2_{Fe}(d)\cdots Na^+$	O $\cdots Na^+$	1.325	0.019
	O $\cdots Na^+$	1.428	0.011
	O $\cdots Na^+$	1.427	0.007
	O $\cdots Na^+$	1.419	0.010
	O $\cdots Na^+$	1.337	0.018
	H ₂ N $\cdots Na^+$	1.287	0.017
$2_{Fe^+}(e)\cdots Na^+$	O $\cdots Na^+$	1.452	0.006
	ONO $\cdots Na^+$	1.467	0.011
	ONO $\cdots Na^+$	1.389	0.016
	ONO $\cdots Na^+$	1.428	0.014
	ONO $\cdots Na^+$	1.403	0.015
$2_{Fe}(e)\cdots Na^+$	O $\cdots Na^+$	1.408	0.012
	O $\cdots Na^+$	1.439	0.012
	ONO $\cdots Na^+$	1.348	0.019
	ONO $\cdots Na^+$	1.385	0.016
	ONO $\cdots Na^+$	1.351	0.019

Table S6. Optimized Cartesian coordinates for the compounds investigated in this study.

1_{OH(a)}Li⁺ / BP86–D3(BJ)/Def2–TZVP

C	-1.168448000	2.090004000	1.667934000
O	-0.796044000	0.708763000	1.715919000
O	-0.552323000	1.975802000	-0.606401000
C	-0.316596000	2.726199000	0.593156000
O	0.471423000	-0.001047000	-2.230325000
C	0.103785000	1.283625000	-2.760283000
C	0.260607000	2.370074000	-1.714497000
O	1.335251000	-1.786516000	-4.070392000
C	2.020702000	-1.722447000	-2.824789000
C	1.865846000	-0.292658000	-2.268670000
C	-1.715351000	-0.139184000	2.408162000
C	-1.384019000	-1.557712000	2.004540000
O	-1.445672000	-1.623043000	0.566689000
C	-1.679919000	-2.959628000	0.085256000
C	-1.923189000	-2.942023000	-1.403962000
O	-0.683387000	-2.855901000	-2.095708000
C	-0.869758000	-2.751118000	-3.509169000
C	0.456101000	-2.912174000	-4.224848000
C	2.439020000	-0.167046000	-0.839553000
C	3.483968000	-2.059866000	-3.135659000
O	1.662444000	-0.200037000	0.135360000
N	3.766545000	-0.028113000	-0.735982000
C	4.472774000	0.040811000	0.536849000
O	4.394308000	-1.253020000	-3.227773000
O	3.630261000	-3.377208000	-3.373258000
H	-0.994382000	2.581930000	2.640113000
H	-2.239083000	2.179736000	1.410933000
H	0.753780000	2.667841000	0.859715000
H	-0.597050000	3.784595000	0.457901000
H	-0.953006000	1.189559000	-3.046356000
H	0.691163000	1.514203000	-3.662701000
H	1.314634000	2.466494000	-1.392822000
H	-0.067762000	3.344837000	-2.117140000
H	1.606981000	-2.443878000	-2.104657000
H	2.385486000	0.397615000	-2.953142000
H	-2.749637000	0.108445000	2.109248000
H	-1.621661000	-0.017963000	3.501390000

H	-2.120984000	-2.247421000	2.448385000
H	-0.376260000	-1.847087000	2.349240000
H	-2.573058000	-3.363477000	0.592391000
H	-0.818243000	-3.607713000	0.322627000
H	-2.580225000	-2.088937000	-1.663258000
H	-2.452567000	-3.871538000	-1.689683000
H	-1.322900000	-1.774874000	-3.762002000
H	-1.551409000	-3.550486000	-3.861130000
H	0.959094000	-3.838489000	-3.902584000
H	0.268892000	-2.980526000	-5.305231000
H	4.302039000	-0.099149000	-1.605470000
H	5.136205000	-0.826885000	0.655630000
H	3.732171000	0.045147000	1.342814000
H	5.075291000	0.957504000	0.586044000
Li	-0.243930000	-0.082983000	-0.129378000
H	4.556233000	-3.524906000	-3.665036000

1_O⁻(a)---Li⁺ / BP86-D3(BJ)/Def2-TZVP

C	-1.857100000	1.835671000	0.378486000
O	-2.146320000	0.507910000	-0.092117000
O	0.530598000	1.893852000	0.334216000
C	-0.587447000	1.841097000	1.196711000
O	3.176574000	0.776034000	-0.639757000
C	2.937282000	1.973592000	0.092345000
C	1.766846000	1.860146000	1.053242000
O	1.212531000	-1.068324000	-0.518246000
C	1.909413000	-0.871270000	-1.782962000
C	2.337473000	0.598302000	-1.795366000
C	-3.395830000	0.450949000	-0.797806000
C	-3.880471000	-0.980260000	-0.763588000
O	-2.855066000	-1.772137000	-1.346463000
C	-2.959174000	-3.176065000	-1.103894000
C	-1.583548000	-3.760440000	-1.329259000
O	-0.712467000	-3.101365000	-0.403843000
C	0.669361000	-3.447233000	-0.561527000
C	1.470466000	-2.332593000	0.088983000
C	3.127007000	1.161496000	-3.003921000
C	0.983621000	-1.267735000	-2.978453000
O	3.466162000	2.350756000	-2.960670000
N	3.453570000	0.311998000	-4.002624000

C	4.162166000	0.788442000	-5.177147000
O	-0.263277000	-1.156049000	-2.760581000
O	1.546288000	-1.663360000	-4.023879000
H	-2.701533000	2.174610000	1.005755000
H	-1.750718000	2.528004000	-0.475072000
H	-0.555560000	0.938861000	1.840770000
H	-0.599659000	2.725990000	1.866290000
H	2.808969000	2.826073000	-0.593572000
H	3.848681000	2.149396000	0.684686000
H	1.840733000	0.914678000	1.623406000
H	1.800218000	2.706097000	1.771336000
H	2.808403000	-1.509055000	-1.788803000
H	1.427268000	1.210163000	-1.699825000
H	-3.256230000	0.795479000	-1.837437000
H	-4.140265000	1.101280000	-0.305911000
H	-4.829417000	-1.073377000	-1.324229000
H	-4.054705000	-1.296997000	0.282182000
H	-3.694334000	-3.639851000	-1.785322000
H	-3.280749000	-3.348757000	-0.060092000
H	-1.245669000	-3.559799000	-2.361072000
H	-1.601254000	-4.850711000	-1.149583000
H	0.915571000	-3.531722000	-1.633880000
H	0.881969000	-4.416854000	-0.073967000
H	1.169747000	-2.228922000	1.142880000
H	2.547902000	-2.567767000	0.055332000
H	2.927672000	-0.582317000	-4.072144000
H	3.471282000	1.182235000	-5.941165000
H	4.735521000	-0.038684000	-5.615576000
H	4.841951000	1.596288000	-4.881674000
Li	-0.874074000	-0.988097000	-1.002303000

1_{OH(a)}···Na⁺ / BP86–D3(BJ)/Def2–TZVP

C	-1.514269000	1.519883000	2.096923000
O	-1.623780000	0.130404000	1.762983000
O	-0.283688000	1.835817000	0.092693000
C	-0.234587000	2.051098000	1.507740000
O	1.087302000	0.462855000	-1.878370000
C	0.885128000	1.890485000	-1.966253000
C	0.810643000	2.477560000	-0.578059000
O	1.100582000	-1.903797000	-3.052530000

C	2.317645000	-1.496095000	-2.443885000
C	2.320451000	0.030434000	-2.436244000
C	-2.901320000	-0.392420000	2.135077000
C	-2.980988000	-1.822772000	1.671806000
O	-2.777633000	-1.844348000	0.251919000
C	-3.084523000	-3.128102000	-0.302357000
C	-2.683828000	-3.131883000	-1.754683000
O	-1.271636000	-2.899075000	-1.828277000
C	-0.695666000	-3.441752000	-3.024871000
C	0.801423000	-3.300354000	-2.942144000
C	3.514677000	0.532264000	-1.580101000
C	3.514895000	-2.015908000	-3.262158000
O	3.402380000	0.633948000	-0.357658000
N	4.632621000	0.817335000	-2.287649000
C	5.888299000	1.212009000	-1.664556000
O	3.978606000	-1.468081000	-4.241841000
O	3.946646000	-3.205288000	-2.784728000
H	-1.512400000	1.654981000	3.193114000
H	-2.378524000	2.067294000	1.678340000
H	0.646857000	1.538632000	1.933352000
H	-0.151635000	3.128808000	1.734055000
H	-0.056890000	2.057260000	-2.513481000
H	1.697742000	2.368477000	-2.533743000
H	1.748812000	2.279145000	-0.036034000
H	0.635989000	3.567839000	-0.632614000
H	2.382821000	-1.887025000	-1.411780000
H	2.401764000	0.378755000	-3.480352000
H	-3.700240000	0.204957000	1.658343000
H	-3.038633000	-0.345260000	3.230403000
H	-3.974444000	-2.232943000	1.924001000
H	-2.212590000	-2.443664000	2.167750000
H	-4.165915000	-3.335040000	-0.208518000
H	-2.529004000	-3.913872000	0.241107000
H	-3.231156000	-2.356981000	-2.321976000
H	-2.935242000	-4.114662000	-2.189552000
H	-1.079936000	-2.913076000	-3.915652000
H	-0.959761000	-4.510950000	-3.112327000
H	1.166460000	-3.699498000	-1.979589000
H	1.279788000	-3.871558000	-3.756076000
H	4.618976000	0.621636000	-3.286618000

H	6.676020000	0.476299000	-1.878425000
H	5.725249000	1.265505000	-0.582946000
H	6.210360000	2.195470000	-2.033339000
Na	-0.734981000	-0.574357000	-0.536127000
H	4.669277000	-3.512257000	-3.375651000

1_o-(a)---Na⁺ / BP86-D3(BJ)/Def2-TZVP

C	-1.973034000	2.129608000	0.098362000
O	-2.420705000	0.774901000	0.188230000
O	0.300783000	1.444740000	0.371032000
C	-0.720640000	2.264225000	0.932276000
O	3.215822000	0.735971000	-0.531890000
C	2.745587000	1.827725000	0.243405000
C	1.543586000	1.496397000	1.119013000
O	1.624181000	-1.395805000	-0.533846000
C	2.214098000	-1.031304000	-1.805913000
C	2.467593000	0.477740000	-1.727592000
C	-3.645521000	0.528666000	-0.505719000
C	-3.946070000	-0.949226000	-0.389062000
O	-2.874298000	-1.647690000	-1.007737000
C	-2.942569000	-3.069156000	-0.875328000
C	-1.634987000	-3.647355000	-1.364641000
O	-0.602780000	-3.224529000	-0.469194000
C	0.698576000	-3.656291000	-0.890525000
C	1.733874000	-2.778925000	-0.205876000
C	3.216950000	1.167013000	-2.898050000
C	1.261782000	-1.370135000	-3.009045000
O	3.489082000	2.367186000	-2.772125000
N	3.548056000	0.410375000	-3.968163000
C	4.184040000	0.991036000	-5.136491000
O	0.026116000	-1.191895000	-2.794582000
O	1.821298000	-1.765777000	-4.059991000
H	-2.746204000	2.818794000	0.486347000
H	-1.766235000	2.394618000	-0.955526000
H	-0.935260000	1.956894000	1.973485000
H	-0.409086000	3.325731000	0.940794000
H	2.541734000	2.703097000	-0.395912000
H	3.579084000	2.087570000	0.915928000
H	1.692422000	0.520242000	1.607608000
H	1.458196000	2.272980000	1.898372000

H	3.167058000	-1.575849000	-1.913824000
H	1.485758000	0.977018000	-1.669463000
H	-3.545043000	0.813202000	-1.569613000
H	-4.468767000	1.117832000	-0.060654000
H	-4.908876000	-1.173459000	-0.886409000
H	-4.029278000	-1.238911000	0.676276000
H	-3.780329000	-3.472449000	-1.473767000
H	-3.105375000	-3.338332000	0.185542000
H	-1.409216000	-3.278182000	-2.381354000
H	-1.709952000	-4.751117000	-1.383607000
H	0.782498000	-3.580919000	-1.986467000
H	0.860407000	-4.712399000	-0.600033000
H	1.598212000	-2.835818000	0.885545000
H	2.744685000	-3.152422000	-0.449233000
H	3.118654000	-0.530089000	-4.062795000
H	3.493414000	1.004452000	-5.994209000
H	5.075750000	0.411301000	-5.416720000
H	4.478009000	2.018861000	-4.894505000
Na	-0.642704000	-0.700481000	-0.709464000

1_{OH(a)}...K⁺ / BP86–D3(BJ)/Def2–TZVP

C	-2.201222000	1.704283000	1.797523000
O	-2.317586000	0.292858000	1.591833000
O	-0.124293000	1.788268000	0.614525000
C	-0.739702000	2.069284000	1.875429000
O	1.830734000	0.463721000	-0.986706000
C	1.831394000	1.886679000	-0.771702000
C	1.254770000	2.174171000	0.589940000
O	1.148470000	-1.826623000	-2.382418000
C	2.515472000	-1.444039000	-2.241100000
C	2.580193000	0.081337000	-2.129935000
C	-3.682157000	-0.130027000	1.520300000
C	-3.721948000	-1.626898000	1.338546000
O	-3.124781000	-1.957591000	0.080750000
C	-3.170014000	-3.362128000	-0.185230000
C	-2.545413000	-3.622945000	-1.533197000
O	-1.159729000	-3.266502000	-1.478344000
C	-0.476248000	-3.563102000	-2.698948000
C	0.988366000	-3.248473000	-2.535571000
C	4.068523000	0.505687000	-1.985385000

C	3.321304000	-1.873222000	-3.482640000
O	4.623507000	0.473171000	-0.891811000
N	4.660794000	0.870689000	-3.151983000
C	6.075937000	1.202524000	-3.245902000
O	3.017594000	-1.579823000	-4.620012000
O	4.397241000	-2.615030000	-3.140606000
H	-2.698521000	1.996312000	2.740488000
H	-2.687175000	2.249452000	0.966843000
H	-0.240917000	1.495482000	2.678718000
H	-0.649029000	3.144904000	2.113741000
H	1.239105000	2.383348000	-1.561947000
H	2.862472000	2.272981000	-0.795529000
H	1.821689000	1.622250000	1.361500000
H	1.349377000	3.255915000	0.796716000
H	2.958240000	-1.894468000	-1.335722000
H	2.134188000	0.513301000	-3.047060000
H	-4.191180000	0.371540000	0.676050000
H	-4.216005000	0.134481000	2.451463000
H	-4.773728000	-1.965806000	1.364117000
H	-3.177354000	-2.127959000	2.160460000
H	-4.216698000	-3.717601000	-0.196828000
H	-2.625276000	-3.916147000	0.602028000
H	-3.059360000	-3.033755000	-2.315245000
H	-2.653567000	-4.694689000	-1.780752000
H	-0.901505000	-2.973365000	-3.532077000
H	-0.584019000	-4.635369000	-2.945107000
H	1.403191000	-3.771250000	-1.654924000
H	1.521891000	-3.597897000	-3.436239000
H	4.102138000	0.862988000	-4.000946000
H	6.562681000	0.590930000	-4.017425000
H	6.532643000	0.996531000	-2.271856000
H	6.216050000	2.264700000	-3.491495000
K	-0.612159000	-0.753755000	-0.399436000
H	4.879761000	-2.831193000	-3.968451000

1_{OH(a)}···K⁺ / ZORA-BP86-D3(BJ)/Def2-TZVP

C	-2.199196000	1.703276000	1.798323000
O	-2.316017000	0.291591000	1.592000000
O	-0.123938000	1.786629000	0.613517000
C	-0.738050000	2.067143000	1.875629000

O	1.831843000	0.461395000	-0.984624000
C	1.831926000	1.885263000	-0.771594000
C	1.255331000	2.173384000	0.589177000
O	1.148579000	-1.826880000	-2.380645000
C	2.516352000	-1.445093000	-2.240330000
C	2.580483000	0.079863000	-2.129113000
C	-3.681613000	-0.129001000	1.518216000
C	-3.723023000	-1.625168000	1.336454000
O	-3.124936000	-1.955831000	0.078615000
C	-3.170774000	-3.360932000	-0.186427000
C	-2.545012000	-3.622448000	-1.532939000
O	-1.158686000	-3.267007000	-1.475872000
C	-0.475144000	-3.563602000	-2.696935000
C	0.988806000	-3.249351000	-2.533345000
C	4.067830000	0.505722000	-1.985547000
C	3.319900000	-1.874706000	-3.482534000
O	4.623343000	0.473270000	-0.892327000
N	4.659057000	0.871396000	-3.152044000
C	6.073242000	1.206321000	-3.245786000
O	3.016848000	-1.578421000	-4.618905000
O	4.395889000	-2.617903000	-3.141817000
H	-2.695682000	1.995005000	2.741778000
H	-2.685216000	2.249147000	0.968200000
H	-0.239023000	1.492529000	2.678120000
H	-0.646691000	3.142534000	2.114567000
H	1.239322000	2.380191000	-1.562543000
H	2.862911000	2.271664000	-0.795282000
H	1.822507000	1.622695000	1.361338000
H	1.349207000	3.255415000	0.794865000
H	2.959693000	-1.895662000	-1.335380000
H	2.132793000	0.511298000	-3.045638000
H	-4.188674000	0.373357000	0.673324000
H	-4.216470000	0.136065000	2.448626000
H	-4.775218000	-1.962764000	1.360852000
H	-3.179700000	-2.126873000	2.158737000
H	-4.217649000	-3.715751000	-0.199436000
H	-2.627571000	-3.914949000	0.601828000
H	-3.057281000	-3.033139000	-2.315908000
H	-2.653552000	-4.694209000	-1.780142000
H	-0.900326000	-2.974041000	-3.530155000

H	-0.582674000	-4.635939000	-2.942908000
H	1.403812000	-3.771783000	-1.652740000
H	1.521931000	-3.598660000	-3.434273000
H	4.100326000	0.864019000	-4.000859000
H	6.562378000	0.593491000	-4.014842000
H	6.529470000	1.004509000	-2.270662000
H	6.210971000	2.268079000	-3.494488000
K	-0.611391000	-0.754755000	-0.398469000
H	4.876894000	-2.832255000	-3.971216000

$1_{\text{O}^-}(\text{a})\cdots\text{K}^+ / \text{BP86-D3(BJ)/Def2-TZVP}$

C	-2.454195000	2.145865000	0.941335000
O	-2.584345000	0.729028000	0.819620000
O	-0.166129000	2.179004000	0.243901000
C	-1.033160000	2.482829000	1.330079000
O	2.157174000	0.802912000	-0.812796000
C	2.051007000	2.221691000	-0.689512000
C	1.199714000	2.534225000	0.516372000
O	1.706023000	-1.666070000	-1.049123000
C	2.248866000	-1.162744000	-2.273837000
C	2.504156000	0.377875000	-2.120239000
C	-3.885013000	0.332668000	0.384762000
C	-3.958779000	-1.176904000	0.361798000
O	-3.043633000	-1.674471000	-0.606758000
C	-3.037488000	-3.105121000	-0.676780000
C	-1.866987000	-3.567642000	-1.512633000
O	-0.661336000	-3.292544000	-0.804486000
C	0.495589000	-3.762112000	-1.514242000
C	1.721876000	-3.085664000	-0.927214000
C	3.953204000	0.743790000	-2.525768000
C	1.334781000	-1.276010000	-3.541227000
O	4.704686000	1.374904000	-1.776544000
N	4.255243000	0.318333000	-3.775950000
C	5.554168000	0.539877000	-4.379004000
O	0.088959000	-1.354522000	-3.340198000
O	1.959288000	-1.158006000	-4.627058000
H	-3.145986000	2.526611000	1.717169000
H	-2.707325000	2.637317000	-0.017438000
H	-0.741347000	1.910754000	2.231969000
H	-0.978010000	3.560943000	1.577780000

H	1.578305000	2.649520000	-1.595705000
H	3.051672000	2.668774000	-0.580073000
H	1.565072000	1.972121000	1.395578000
H	1.263208000	3.615468000	0.741570000
H	3.204664000	-1.679308000	-2.464252000
H	1.842245000	0.904086000	-2.838644000
H	-4.091064000	0.741298000	-0.623261000
H	-4.657357000	0.720332000	1.076516000
H	-4.994888000	-1.480579000	0.114673000
H	-3.711587000	-1.581763000	1.361873000
H	-3.982175000	-3.463474000	-1.127630000
H	-2.954689000	-3.525990000	0.342726000
H	-1.852326000	-3.055641000	-2.492793000
H	-1.976483000	-4.655605000	-1.690952000
H	0.392257000	-3.521111000	-2.582796000
H	0.589818000	-4.859642000	-1.391201000
H	1.770726000	-3.290300000	0.153999000
H	2.628548000	-3.507334000	-1.399098000
H	3.530941000	-0.241264000	-4.274200000
H	5.461135000	1.113083000	-5.314058000
H	6.053610000	-0.414832000	-4.605462000
H	6.169360000	1.106429000	-3.669463000
K	-0.601620000	-0.381424000	-0.918433000

$1_{\text{O}}^-(\text{a})\cdots\text{K}^+ / \text{ZORA-BP86-D3(BJ)/Def2-TZVP}$

C	-2.453915000	2.145732000	0.940991000
O	-2.584007000	0.728696000	0.819467000
O	-0.166092000	2.179026000	0.243319000
C	-1.033023000	2.482502000	1.329847000
O	2.156916000	0.802730000	-0.812435000
C	2.050990000	2.221699000	-0.689504000
C	1.199809000	2.534323000	0.516133000
O	1.706048000	-1.666005000	-1.048830000
C	2.249081000	-1.162689000	-2.273729000
C	2.504211000	0.377762000	-2.120028000
C	-3.884770000	0.332586000	0.384353000
C	-3.958498000	-1.176721000	0.361553000
O	-3.043389000	-1.674248000	-0.607223000
C	-3.037360000	-3.105073000	-0.676516000
C	-1.867161000	-3.567726000	-1.512289000

O	-0.661436000	-3.292572000	-0.803973000
C	0.495335000	-3.761950000	-1.514339000
C	1.721518000	-3.085750000	-0.927431000
C	3.953181000	0.743568000	-2.525358000
C	1.335244000	-1.276335000	-3.540931000
O	4.705012000	1.373683000	-1.775726000
N	4.254865000	0.318740000	-3.775683000
C	5.553580000	0.540309000	-4.378889000
O	0.089400000	-1.354800000	-3.340091000
O	1.959935000	-1.158617000	-4.626739000
H	-3.145676000	2.526713000	1.716709000
H	-2.706827000	2.637070000	-0.017885000
H	-0.741322000	1.909893000	2.231429000
H	-0.977867000	3.560460000	1.578098000
H	1.578323000	2.649536000	-1.595716000
H	3.051720000	2.668551000	-0.580009000
H	1.565073000	1.972355000	1.395453000
H	1.263357000	3.615624000	0.741078000
H	3.204934000	-1.679072000	-2.464098000
H	1.842386000	0.903945000	-2.838443000
H	-4.090828000	0.741269000	-0.623615000
H	-4.657163000	0.720001000	1.076183000
H	-4.994608000	-1.480383000	0.114527000
H	-3.711149000	-1.581298000	1.361690000
H	-3.982037000	-3.463552000	-1.127236000
H	-2.954456000	-3.525523000	0.343144000
H	-1.852554000	-3.055884000	-2.492448000
H	-1.976828000	-4.655711000	-1.690289000
H	0.391729000	-3.520401000	-2.582731000
H	0.589520000	-4.859510000	-1.391678000
H	1.770329000	-3.290439000	0.153771000
H	2.628160000	-3.507337000	-1.399410000
H	3.530179000	-0.239966000	-4.274236000
H	5.460173000	1.113723000	-5.313790000
H	6.052949000	-0.414372000	-4.605680000
H	6.168870000	1.106690000	-3.669297000
K	-0.601489000	-0.381590000	-0.918580000

$1_{\text{OH}(b)} \cdots \text{Na}^+ / \text{BP86-D3(BJ)/Def2-TZVP}$

C	-1.740412000	1.294944000	2.399694000
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O	-1.770306000	-0.117041000	2.130341000
O	-0.020561000	1.480489000	0.756720000
C	-0.293393000	1.743179000	2.168308000
O	1.416508000	0.499855000	-1.195498000
C	0.996981000	1.941026000	-1.316484000
C	0.914565000	2.392599000	0.151010000
O	1.086441000	-2.102303000	-1.883601000
C	2.388470000	-1.508898000	-1.956619000
C	2.258037000	-0.002380000	-2.204000000
C	-3.161505000	-0.631095000	1.991692000
C	-3.074783000	-1.984667000	1.286458000
O	-2.432000000	-1.810226000	-0.011019000
C	-3.081317000	-2.487141000	-1.150600000
C	-1.929287000	-2.870184000	-2.097785000
O	-1.288399000	-3.969595000	-1.420841000
C	0.057455000	-4.282652000	-1.863356000
C	1.053561000	-3.353508000	-1.132347000
C	3.684792000	0.608889000	-2.099643000
C	3.120602000	-2.183767000	-3.128022000
O	4.129714000	0.980245000	-1.008271000
N	4.372526000	0.663615000	-3.262172000
C	5.757092000	1.108933000	-3.346504000
O	3.070755000	-1.815323000	-4.285315000
O	3.775215000	-3.295030000	-2.720700000
H	-2.386489000	1.809357000	1.665729000
H	-0.235500000	2.834443000	2.314515000
H	-0.003891000	1.917434000	-1.775189000
H	0.483892000	3.407935000	0.172234000
H	2.935234000	-1.667076000	-1.012103000
H	1.837905000	0.156943000	-3.213458000
H	-3.669809000	0.092596000	1.330917000
H	-4.099836000	-2.329336000	1.114457000
H	-3.725125000	-1.741164000	-1.644100000
H	-1.238020000	-2.018713000	-2.195983000
H	0.113704000	-4.102658000	-2.946577000
H	2.047663000	-3.814359000	-1.173442000
H	3.942761000	0.237429000	-4.081658000
H	6.412945000	0.284804000	-3.660417000
H	6.062447000	1.454162000	-2.353246000
H	5.853004000	1.933128000	-4.066329000

Na	-0.274349000	-0.718763000	0.127286000
H	4.145671000	-3.730273000	-3.519895000
N	1.819868000	2.813159000	-2.050659000
H	1.804528000	2.714550000	-3.060335000
H	2.759108000	2.934486000	-1.677632000
N	2.183154000	2.406426000	0.832126000
H	2.589261000	3.337712000	0.887715000
H	2.857700000	1.746964000	0.421721000
N	0.588075000	1.111549000	3.100212000
H	1.550418000	1.400568000	2.915970000
H	0.515464000	0.094291000	3.055627000
N	-2.230995000	1.605116000	3.729890000
H	-2.569525000	2.566756000	3.778819000
H	-1.475775000	1.490316000	4.412436000
N	-3.890152000	-0.787771000	3.199238000
H	-3.812864000	0.057774000	3.768822000
H	-3.539287000	-1.593877000	3.720588000
N	-2.433487000	-2.948941000	2.133282000
H	-1.472100000	-2.703772000	2.366572000
H	-2.492911000	-3.892970000	1.756574000
N	-3.865245000	-3.615735000	-0.770262000
H	-3.394655000	-4.510531000	-0.884280000
H	-4.825933000	-3.621308000	-1.092477000
N	-2.315656000	-3.276548000	-3.424335000
H	-2.402817000	-2.491654000	-4.068102000
H	-3.183151000	-3.816486000	-3.423292000
N	0.385413000	-5.643617000	-1.586528000
H	-0.205953000	-6.280998000	-2.120023000
H	0.284938000	-5.866916000	-0.594205000
N	0.664255000	-3.086179000	0.239450000
H	1.301756000	-3.494963000	0.919761000
H	-0.294424000	-3.420620000	0.394889000

$1_{\text{O}^-}(\text{b}) \cdots \text{Na}^+ / \text{BP86-D3(BJ)/Def2-TZVP}$

C	-1.989727000	1.366598000	2.164388000
O	-1.884900000	-0.049061000	2.258626000
O	-0.228537000	1.404724000	0.514352000
C	-0.586384000	1.879387000	1.844209000
O	1.567564000	0.479377000	-1.171671000
C	0.938511000	1.751786000	-1.537147000

C	0.590635000	2.376661000	-0.179160000
O	1.280076000	-1.924283000	-2.153994000
C	2.629309000	-1.521030000	-1.766527000
C	2.623107000	-0.013973000	-1.992417000
C	-3.184945000	-0.709689000	2.346178000
C	-2.979317000	-2.103720000	1.767221000
O	-2.568234000	-1.940905000	0.368588000
C	-3.234768000	-2.847983000	-0.516020000
C	-2.525517000	-2.709823000	-1.878842000
O	-1.201088000	-3.156286000	-1.585208000
C	-0.338517000	-3.549644000	-2.708558000
C	1.088291000	-3.344065000	-2.209364000
C	3.965089000	0.679315000	-1.622357000
C	3.697079000	-2.359681000	-2.563187000
O	4.045371000	1.462738000	-0.655590000
N	4.974459000	0.387126000	-2.453610000
C	6.326934000	0.865045000	-2.238213000
O	4.144559000	-1.853253000	-3.634534000
O	3.948589000	-3.478552000	-2.056033000
H	-2.668441000	1.629121000	1.331486000
H	-0.632807000	2.980477000	1.792992000
H	0.018703000	1.515575000	-2.102582000
H	-0.018495000	3.280130000	-0.360109000
H	2.766914000	-1.727498000	-0.690257000
H	2.417416000	0.148520000	-3.063887000
H	-3.871023000	-0.144721000	1.691547000
H	-3.944705000	-2.626613000	1.777053000
H	-4.293943000	-2.547861000	-0.624617000
H	-2.504252000	-1.649689000	-2.193433000
H	-0.522315000	-2.851212000	-3.537847000
H	1.770363000	-3.762889000	-2.964924000
H	4.782277000	-0.402812000	-3.122933000
H	6.985340000	0.042661000	-1.919016000
H	6.311083000	1.634432000	-1.457542000
H	6.731604000	1.291647000	-3.167155000
Na	-0.107506000	-1.141031000	-0.292433000
N	1.705563000	2.678858000	-2.300612000
H	1.842742000	2.384717000	-3.265349000
H	2.612285000	2.856694000	-1.861650000
N	1.754122000	2.742795000	0.595104000

H	1.988674000	3.725223000	0.463764000
H	2.570535000	2.163559000	0.329550000
N	0.321426000	1.523347000	2.896646000
H	1.245832000	1.887145000	2.650322000
H	0.368219000	0.508094000	2.996221000
N	-2.533917000	1.938109000	3.393080000
H	-2.941113000	2.856391000	3.208824000
H	-1.761600000	2.058889000	4.057915000
N	-3.750186000	-0.809036000	3.655641000
H	-3.747469000	0.119799000	4.084683000
H	-3.189758000	-1.451466000	4.220642000
N	-2.054587000	-2.851887000	2.562617000
H	-1.143399000	-2.393750000	2.605326000
H	-1.952899000	-3.795108000	2.188829000
N	-3.195293000	-4.209660000	-0.022290000
H	-2.375196000	-4.706554000	-0.373690000
H	-4.051154000	-4.735467000	-0.177368000
N	-3.168117000	-3.470252000	-2.933819000
H	-3.770784000	-2.885897000	-3.509936000
H	-3.714092000	-4.248044000	-2.556644000
N	-0.528271000	-4.883285000	-3.179900000
H	-1.489539000	-5.016662000	-3.489876000
H	-0.267280000	-5.593555000	-2.496010000
N	1.325642000	-3.904387000	-0.883858000
H	2.327515000	-4.143683000	-0.849969000
H	0.766467000	-4.740187000	-0.711479000

1_{OH(c)}...Na⁺ / BP86-D3(BJ)/Def2-TZVP

C	-2.104610000	1.846796000	2.091325000
O	-2.664334000	0.575174000	2.184136000
O	-0.055327000	1.046744000	1.246911000
C	-0.594698000	1.748268000	2.329016000
O	1.290386000	-0.066265000	-1.086710000
C	1.428902000	1.225491000	-0.603094000
C	1.279510000	1.344975000	0.905870000
O	1.246914000	-2.471491000	-2.388343000
C	2.449270000	-1.653088000	-2.432555000
C	1.977144000	-0.208824000	-2.359186000
C	-3.369040000	0.048760000	1.110970000
C	-3.384263000	-1.471642000	1.239764000

O	-2.216688000	-1.982303000	0.651137000
C	-2.356819000	-3.149479000	-0.108027000
C	-1.376057000	-3.058444000	-1.288315000
O	-1.002765000	-4.333140000	-1.664021000
C	0.130790000	-4.537331000	-2.477498000
C	1.404902000	-3.799587000	-2.049051000
C	3.162776000	0.772021000	-2.439084000
C	3.150983000	-1.934868000	-3.767779000
O	4.348593000	0.336025000	-1.840744000
N	3.309925000	1.429510000	-3.617027000
C	4.483414000	2.261758000	-3.905614000
O	2.987947000	-1.285721000	-4.778340000
O	3.918453000	-3.041030000	-3.672958000
H	-2.298124000	2.350053000	1.135678000
H	-0.146811000	2.738145000	2.490638000
H	0.699317000	1.931099000	-1.049920000
H	1.583488000	2.358321000	1.209109000
H	3.102020000	-1.872851000	-1.576492000
H	1.266011000	-0.004808000	-3.176286000
H	-2.944190000	0.310372000	0.128962000
H	-4.305643000	-1.883160000	0.808371000
H	-3.391650000	-3.342705000	-0.418736000
H	-0.542841000	-2.387926000	-1.031419000
H	-0.076817000	-4.298086000	-3.528618000
H	2.292230000	-4.289078000	-2.475574000
H	2.822548000	1.029703000	-4.415435000
H	5.272710000	1.688467000	-4.412209000
H	4.879792000	2.662478000	-2.968155000
H	4.174727000	3.097832000	-4.544234000
Na	0.023065000	-2.150136000	2.173091000
H	4.308439000	-3.222955000	-4.556950000
N	2.774072000	1.740842000	-1.080478000
O	3.960449000	0.518632000	-0.442915000
O	3.034241000	2.922663000	-0.935906000
N	2.256439000	0.404770000	1.677580000
O	1.933649000	-0.778113000	1.786179000
O	3.250838000	0.936930000	2.132644000
N	-0.371389000	0.980518000	3.682380000
O	-0.172148000	-0.231744000	3.629033000
O	-0.446694000	1.667763000	4.681736000

N	-2.718854000	2.801704000	3.174077000
O	-3.450411000	2.318118000	4.009751000
O	-2.354959000	3.964238000	3.039101000
N	-4.835276000	0.620422000	1.032487000
O	-5.658178000	-0.077075000	0.459200000
O	-4.975624000	1.747508000	1.475933000
N	-3.427232000	-1.831043000	2.760992000
O	-4.480357000	-1.570516000	3.309373000
O	-2.416558000	-2.318014000	3.257215000
N	-1.967003000	-4.400238000	0.756598000
O	-2.648994000	-5.390536000	0.605418000
O	-0.998698000	-4.263174000	1.506689000
N	-2.103826000	-2.295645000	-2.454910000
O	-1.984820000	-2.753984000	-3.576660000
O	-2.695959000	-1.269420000	-2.126345000
N	0.401775000	-6.070061000	-2.458356000
O	-0.285738000	-6.767687000	-1.742210000
O	1.302767000	-6.403798000	-3.219647000
N	1.575112000	-3.981705000	-0.487873000
O	1.953841000	-5.073666000	-0.116004000
O	1.295038000	-3.009847000	0.218921000

1_o⁻(c)---Na⁺ / BP86-D3(BJ)/Def2-TZVP

C	-1.766937000	1.825601000	2.331473000
O	-2.532871000	0.690823000	2.073911000
O	0.165863000	0.563200000	1.905059000
C	-0.404610000	1.379893000	2.884296000
O	2.629010000	0.537190000	-0.623093000
C	1.402637000	0.665723000	-0.081211000
C	1.456152000	0.855091000	1.441156000
O	1.629613000	-1.838377000	-1.310136000
C	2.046385000	-1.080994000	-2.478356000
C	2.583989000	0.327020000	-2.051123000
C	-2.894833000	0.410963000	0.757647000
C	-3.268973000	-1.063342000	0.644532000
O	-2.135728000	-1.814671000	0.296749000
C	-2.429278000	-3.024191000	-0.381177000
C	-1.544524000	-3.205976000	-1.609845000
O	-0.434033000	-3.966835000	-1.268255000
C	0.677146000	-3.921747000	-2.118454000

C	1.850888000	-3.196096000	-1.422059000
C	4.014064000	0.555702000	-2.594787000
C	0.920124000	-0.855828000	-3.536530000
O	4.983850000	0.644027000	-1.848854000
N	4.015801000	0.606807000	-3.946772000
C	5.237794000	0.734441000	-4.719817000
O	1.297138000	-0.146688000	-4.496215000
O	-0.214968000	-1.365103000	-3.319871000
H	-1.604709000	2.458926000	1.450257000
H	0.215441000	2.233670000	3.184516000
H	0.667299000	-0.106407000	-0.352220000
H	1.818194000	1.854305000	1.720586000
H	2.867183000	-1.633617000	-2.964498000
H	1.925814000	1.088692000	-2.494800000
H	-2.105460000	0.653388000	0.027966000
H	-4.094536000	-1.189234000	-0.067658000
H	-3.483312000	-3.076430000	-0.680831000
H	-1.253275000	-2.238081000	-2.081614000
H	0.467890000	-3.406601000	-3.065711000
H	2.802920000	-3.455116000	-1.909975000
H	3.104935000	0.447482000	-4.412688000
H	5.372962000	-0.132113000	-5.383528000
H	6.080743000	0.789855000	-4.021265000
H	5.217651000	1.646968000	-5.333019000
Na	-0.271050000	-2.153804000	2.197577000
N	0.673070000	2.032994000	-0.568821000
O	1.377061000	2.998415000	-0.787315000
O	-0.561366000	1.991376000	-0.642346000
N	2.488118000	-0.113213000	2.103192000
O	2.036742000	-1.131181000	2.627788000
O	3.646117000	0.246013000	2.057766000
N	-0.624999000	0.546049000	4.185330000
O	-0.607867000	-0.678471000	4.096030000
O	-0.827498000	1.205365000	5.189084000
N	-2.476087000	2.746165000	3.365646000
O	-3.476145000	2.333996000	3.915175000
O	-1.902722000	3.820982000	3.517196000
N	-4.102316000	1.312840000	0.303629000
O	-4.746616000	0.910815000	-0.653469000
O	-4.226332000	2.369288000	0.902737000

N	-3.845636000	-1.504098000	2.034171000
O	-4.987241000	-1.132780000	2.249228000
O	-3.110906000	-2.146123000	2.774509000
N	-2.208031000	-4.247463000	0.556674000
O	-2.798968000	-5.256172000	0.218356000
O	-1.445559000	-4.124940000	1.512398000
N	-2.394752000	-3.904702000	-2.731642000
O	-1.811636000	-4.718412000	-3.426313000
O	-3.548604000	-3.503570000	-2.857711000
N	1.102654000	-5.362552000	-2.478994000
O	2.043385000	-5.404918000	-3.270800000
O	0.509523000	-6.296484000	-1.972889000
N	1.940230000	-3.774243000	0.005161000
O	1.413864000	-3.131377000	0.914652000
O	2.489397000	-4.855997000	0.115245000

1_{OH}(a) / BP86–D3(BJ)/Def2–TZVP

C	-0.819434000	1.248445000	2.073693000
O	-0.684089000	0.782756000	0.735943000
O	1.565140000	0.988317000	2.705258000
C	0.221858000	0.587360000	2.959985000
O	2.861300000	0.507423000	-0.723277000
C	2.451059000	1.255723000	0.434949000
C	2.203314000	0.313762000	1.617251000
O	1.119585000	-2.313677000	-2.185808000
C	2.122455000	-1.685148000	-1.416928000
C	1.780678000	-0.179461000	-1.358842000
C	-1.582634000	1.419072000	-0.192016000
C	-2.865949000	0.627874000	-0.424414000
O	-2.740721000	-0.411090000	-1.390026000
C	-2.041855000	-1.569870000	-0.943427000
C	-1.974277000	-2.511904000	-2.136686000
O	-1.406837000	-3.765395000	-1.731241000
C	-0.304520000	-4.217325000	-2.504499000
C	1.031115000	-3.726810000	-1.975708000
C	1.433802000	0.564414000	-2.666196000
C	3.523984000	-1.974287000	-1.967003000
O	0.744797000	1.587963000	-2.578123000
N	1.944782000	0.092319000	-3.824989000
C	1.710530000	0.750334000	-5.097232000

O	3.811306000	-2.037632000	-3.150545000
O	4.421785000	-2.181722000	-0.979286000
H	-1.824868000	1.010791000	2.478413000
H	-0.691298000	2.347993000	2.105209000
H	0.128156000	-0.512292000	2.881172000
H	0.013268000	0.872816000	4.002860000
H	1.542072000	1.834897000	0.217175000
H	3.274571000	1.949579000	0.649369000
H	1.580376000	-0.531533000	1.280888000
H	3.161438000	-0.093025000	1.980576000
H	2.105747000	-2.054880000	-0.375412000
H	0.867544000	-0.105177000	-0.748079000
H	-1.029675000	1.525124000	-1.138770000
H	-1.830783000	2.431819000	0.175098000
H	-3.630833000	1.305992000	-0.833376000
H	-3.246665000	0.221493000	0.534733000
H	-2.580703000	-2.051132000	-0.103090000
H	-1.023788000	-1.327479000	-0.597044000
H	-1.373874000	-2.043682000	-2.930677000
H	-2.993036000	-2.687752000	-2.523705000
H	-0.416120000	-3.926269000	-3.564438000
H	-0.309377000	-5.318191000	-2.453820000
H	1.101645000	-3.947508000	-0.894333000
H	1.857741000	-4.246685000	-2.498093000
H	2.501354000	-0.765397000	-3.809044000
H	2.662574000	1.024603000	-5.575002000
H	1.126309000	1.657170000	-4.905155000
H	1.148108000	0.095880000	-5.780314000
H	5.292540000	-2.307230000	-1.414460000

$1_{\text{O}}^{-}(\text{a}) / \text{BP86-D3(BJ)/Def2-TZVP}$

C	-1.604731000	2.244846000	0.019910000
O	-2.883884000	1.927804000	-0.532789000
O	-0.122349000	1.643368000	1.912237000
C	-1.437078000	1.533226000	1.369120000
O	2.582153000	0.568827000	-0.364265000
C	1.867036000	1.491080000	0.459797000
C	0.818743000	0.749229000	1.297503000
O	1.133985000	-1.773745000	-0.706169000
C	1.938942000	-1.270972000	-1.784007000

C	1.905080000	0.251824000	-1.601912000
C	-2.836542000	1.068611000	-1.677354000
C	-2.152588000	-0.271916000	-1.487535000
O	-2.888002000	-1.083161000	-0.568411000
C	-2.086199000	-2.133710000	-0.019961000
C	-1.676074000	-3.178746000	-1.057815000
O	-0.826511000	-4.161223000	-0.437804000
C	0.515631000	-4.173069000	-0.933017000
C	1.414267000	-3.108362000	-0.305610000
C	2.514557000	1.197071000	-2.662170000
C	1.451194000	-1.746158000	-3.205485000
O	2.296152000	2.414434000	-2.549213000
N	3.315947000	0.641575000	-3.597784000
C	3.892525000	1.451231000	-4.651728000
O	0.235099000	-1.999564000	-3.351989000
O	2.380271000	-1.819672000	-4.070924000
H	-1.549732000	3.337925000	0.156552000
H	-0.790949000	1.963602000	-0.668955000
H	-1.731567000	0.475529000	1.249196000
H	-2.118285000	1.984875000	2.106769000
H	1.399137000	2.278123000	-0.152422000
H	2.614795000	1.976260000	1.105561000
H	0.308759000	0.016565000	0.652191000
H	1.315546000	0.175793000	2.097835000
H	2.978820000	-1.620219000	-1.646223000
H	0.841040000	0.535126000	-1.528138000
H	-2.325766000	1.583994000	-2.515464000
H	-3.888748000	0.910852000	-1.957780000
H	-1.117734000	-0.141740000	-1.123625000
H	-2.054262000	-0.757106000	-2.475130000
H	-2.692332000	-2.592274000	0.776108000
H	-1.168961000	-1.715673000	0.436135000
H	-1.147883000	-2.697507000	-1.897220000
H	-2.573979000	-3.696507000	-1.440617000
H	0.523318000	-4.077750000	-2.030899000
H	0.922795000	-5.161295000	-0.655544000
H	1.278513000	-3.140096000	0.789824000
H	2.471331000	-3.356340000	-0.527933000
H	3.184572000	-0.389612000	-3.778232000
H	3.361940000	1.299201000	-5.606712000

H	4.951344000	1.188989000	-4.800909000
H	3.812656000	2.507539000	-4.365668000

1_{OH}(b) / BP86–D3(BJ)/Def2–TZVP

C	-0.820537000	0.649714000	2.984377000
O	-1.935116000	0.079829000	2.257627000
O	0.856805000	0.598136000	1.193819000
C	0.504276000	0.034985000	2.491567000
O	2.625894000	1.110287000	-0.900358000
C	1.850794000	2.156727000	-0.244935000
C	1.703312000	1.752717000	1.233868000
O	1.476652000	-2.218460000	-1.662905000
C	2.374828000	-1.272322000	-1.111041000
C	1.874015000	0.120497000	-1.566738000
C	-2.298024000	0.711831000	1.001333000
C	-3.108622000	-0.346517000	0.242636000
O	-2.154692000	-1.333817000	-0.268853000
C	-2.640085000	-2.029090000	-1.401976000
C	-1.423686000	-2.601888000	-2.160366000
O	-0.918847000	-3.683877000	-1.369412000
C	0.336114000	-4.260376000	-1.833812000
C	1.503386000	-3.556996000	-1.117753000
C	1.873540000	0.440020000	-3.086910000
C	3.811122000	-1.576697000	-1.535407000
O	1.912424000	1.613958000	-3.458327000
N	1.759441000	-0.622399000	-3.924598000
C	1.750011000	-0.477566000	-5.367937000
O	4.130226000	-2.289534000	-2.466694000
O	4.713837000	-0.964587000	-0.725226000
H	-0.808331000	1.741503000	2.814379000
H	1.315710000	0.283860000	3.189977000
H	0.860892000	2.204084000	-0.723212000
H	1.222531000	2.579631000	1.788126000
H	2.318093000	-1.271661000	-0.012488000
H	0.819505000	0.139764000	-1.238598000
H	-1.382823000	0.941163000	0.439598000
H	-3.566291000	0.136941000	-0.637476000
H	-3.129889000	-1.313396000	-2.093319000
H	-0.672834000	-1.804349000	-2.247172000
H	0.404541000	-4.099903000	-2.918879000

H	2.451011000	-4.044531000	-1.396090000
H	1.788512000	-1.553968000	-3.509989000
H	2.708610000	-0.793212000	-5.808516000
H	1.585667000	0.580568000	-5.601634000
H	0.944923000	-1.081984000	-5.809506000
H	5.596724000	-1.183361000	-1.092619000
N	2.491128000	3.425175000	-0.375433000
H	2.605998000	3.634333000	-1.369787000
H	3.423333000	3.393719000	0.044894000
N	2.961438000	1.440076000	1.879281000
H	3.388280000	2.248503000	2.327010000
H	3.608271000	1.010972000	1.212569000
N	0.342862000	-1.382072000	2.403859000
H	1.178160000	-1.822072000	2.012600000
H	-0.444864000	-1.578815000	1.777673000
N	-0.954051000	0.392870000	4.390152000
H	-0.846183000	-0.613126000	4.547445000
H	-1.882757000	0.668634000	4.713451000
N	-3.093135000	1.905077000	1.133239000
H	-2.582309000	2.652208000	1.603376000
H	-3.945541000	1.694242000	1.657897000
N	-4.147414000	-0.860428000	1.087837000
H	-3.725474000	-1.209981000	1.951320000
H	-4.611754000	-1.638654000	0.614455000
N	-3.654137000	-3.017824000	-1.029015000
H	-3.192871000	-3.861736000	-0.678508000
H	-4.237190000	-3.271961000	-1.827791000
N	-1.727092000	-3.085016000	-3.498969000
H	-1.801413000	-2.312199000	-4.161257000
H	-2.604370000	-3.611860000	-3.510696000
N	0.388732000	-5.665187000	-1.560064000
H	-0.347419000	-6.153808000	-2.070344000
H	0.248062000	-5.840888000	-0.562326000
N	1.379161000	-3.537670000	0.316324000
H	1.894214000	-4.288390000	0.769356000
H	0.396606000	-3.541766000	0.598075000

$1_{\text{O}}^-(\text{b}) / \text{BP86-D3(BJ)/Def2-TZVP}$

C	-2.928726000	1.300040000	1.584133000
O	-2.820693000	0.464210000	2.764983000

O	-0.678934000	1.114644000	0.773774000
C	-1.588669000	2.034590000	1.420057000
O	1.524431000	-0.065923000	-0.880884000
C	0.978774000	1.270465000	-1.002684000
C	0.556442000	1.726555000	0.420582000
O	1.082551000	-2.090608000	-2.599196000
C	2.419669000	-1.940289000	-2.066284000
C	2.534057000	-0.430276000	-1.815517000
C	-3.341453000	-0.884402000	2.687888000
C	-2.290374000	-1.842591000	2.101286000
O	-2.258623000	-1.588310000	0.681303000
C	-1.607851000	-2.602850000	-0.078049000
C	-1.879677000	-2.286025000	-1.566969000
O	-1.559901000	-3.489252000	-2.264694000
C	-0.737325000	-3.341401000	-3.446120000
C	0.755616000	-3.399160000	-3.080101000
C	3.919948000	0.068895000	-1.297955000
C	3.455409000	-2.561393000	-3.084072000
O	4.040265000	0.645183000	-0.200450000
N	4.928827000	-0.112671000	-2.168521000
C	6.293888000	0.252161000	-1.859782000
O	3.945611000	-1.785355000	-3.964784000
O	3.651030000	-3.794507000	-2.959163000
H	-3.092073000	0.660245000	0.707023000
H	-1.738666000	2.885855000	0.733006000
H	0.074526000	1.214703000	-1.635194000
H	0.413631000	2.820633000	0.331455000
H	2.495115000	-2.486238000	-1.110675000
H	2.359090000	0.037163000	-2.800508000
H	-4.235954000	-0.881525000	2.039560000
H	-2.635471000	-2.883062000	2.249187000
H	-2.073674000	-3.587044000	0.148695000
H	-1.202154000	-1.469078000	-1.863592000
H	-0.948213000	-2.357634000	-3.894812000
H	1.336015000	-3.583002000	-4.002453000
H	4.688621000	-0.678379000	-3.026840000
H	6.936430000	-0.640969000	-1.800688000
H	6.307628000	0.769081000	-0.891880000
H	6.704773000	0.919348000	-2.634190000
N	1.843315000	2.286609000	-1.559909000

H	2.024117000	2.117155000	-2.548873000
H	2.746504000	2.282970000	-1.075970000
N	1.536236000	1.460738000	1.474645000
H	2.483612000	1.564175000	1.083008000
H	1.483534000	0.450200000	1.643877000
N	-1.164217000	2.549455000	2.700986000
H	-0.197677000	2.880393000	2.630981000
H	-1.159920000	1.769994000	3.365783000
N	-3.985135000	2.283754000	1.690995000
H	-3.772110000	2.891712000	2.487763000
H	-4.876095000	1.820988000	1.880354000
N	-3.683680000	-1.345551000	4.006679000
H	-4.198710000	-0.613574000	4.499579000
H	-2.803441000	-1.504900000	4.509480000
N	-1.049052000	-1.664133000	2.813461000
H	-0.750936000	-0.694691000	2.660196000
H	-0.353908000	-2.258405000	2.343308000
N	-0.190502000	-2.690037000	0.246298000
H	0.259654000	-1.816817000	-0.062766000
H	0.239433000	-3.426149000	-0.338604000
N	-3.244783000	-1.901282000	-1.920771000
H	-3.465259000	-1.036182000	-1.418328000
H	-3.884742000	-2.611230000	-1.547940000
N	-1.052754000	-4.372525000	-4.402335000
H	-2.067994000	-4.433765000	-4.499628000
H	-0.721176000	-5.281286000	-4.069417000
N	1.021342000	-4.413870000	-2.071669000
H	1.983696000	-4.748441000	-2.204151000
H	0.333972000	-5.166174000	-2.086236000

$1_{\text{OH}(c)}$ / BP86–D3(BJ)/Def2–TZVP

C	-1.659370000	1.664788000	2.562701000
O	-2.475637000	0.574696000	2.205218000
O	0.275904000	1.095760000	1.367189000
C	-0.150947000	1.398779000	2.656127000
O	0.893903000	0.428494000	-1.200418000
C	1.172293000	1.692023000	-0.672984000
C	1.459049000	1.642615000	0.831334000
O	0.997717000	-2.214756000	-2.048138000
C	2.170522000	-1.360450000	-2.140962000

C	1.674662000	0.066480000	-2.350762000
C	-2.139157000	-0.262057000	1.154254000
C	-3.055035000	-1.497427000	1.159138000
O	-2.390295000	-2.516805000	0.476937000
C	-3.029956000	-3.130377000	-0.586987000
C	-1.983896000	-3.393030000	-1.666106000
O	-1.090939000	-4.349508000	-1.209562000
C	0.155115000	-4.424383000	-1.845246000
C	1.186282000	-3.399484000	-1.348175000
C	2.810872000	1.083252000	-2.516778000
C	2.961846000	-1.854264000	-3.356154000
O	3.953541000	0.888229000	-1.685277000
N	3.077205000	1.446429000	-3.798493000
C	4.226843000	2.273646000	-4.156713000
O	2.821212000	-1.444839000	-4.491574000
O	3.788160000	-2.864859000	-3.008810000
H	-1.802766000	2.502886000	1.868271000
H	0.356518000	2.261118000	3.112114000
H	0.306382000	2.364194000	-0.799373000
H	1.679279000	2.646482000	1.221704000
H	2.761751000	-1.408984000	-1.217858000
H	1.022787000	0.097223000	-3.239014000
H	-1.092435000	-0.597922000	1.127392000
H	-4.064899000	-1.296730000	0.778827000
H	-3.857179000	-2.545541000	-1.012602000
H	-1.517533000	-2.428418000	-1.918777000
H	0.074630000	-4.348979000	-2.937936000
H	2.201032000	-3.811401000	-1.431467000
H	2.664902000	0.869239000	-4.526289000
H	3.923231000	3.019331000	-4.902400000
H	5.048579000	1.665544000	-4.563303000
H	4.584875000	2.799025000	-3.266429000
H	4.205940000	-3.207518000	-3.828968000
N	2.262076000	2.319164000	-1.531915000
O	3.740607000	1.974524000	-0.715625000
O	2.107445000	3.470192000	-1.918169000
N	2.648072000	0.770548000	1.321738000
O	2.853017000	-0.312735000	0.798294000
O	3.218339000	1.233705000	2.308066000
N	0.149079000	0.202749000	3.629941000

O	0.879123000	-0.681680000	3.224966000
O	-0.377832000	0.310215000	4.730312000
N	-2.204563000	2.206639000	3.908118000
O	-3.162472000	1.660516000	4.413087000
O	-1.612820000	3.213158000	4.293885000
N	-2.332408000	0.466850000	-0.230661000
O	-2.424419000	-0.240734000	-1.228603000
O	-2.348407000	1.691518000	-0.217523000
N	-3.253134000	-1.936058000	2.644478000
O	-4.384143000	-1.803694000	3.089807000
O	-2.258344000	-2.356773000	3.212730000
N	-3.694280000	-4.468037000	-0.112425000
O	-3.973041000	-5.260400000	-1.003745000
O	-3.924254000	-4.568450000	1.080750000
N	-2.677293000	-3.820621000	-3.007102000
O	-2.176604000	-4.750636000	-3.620790000
O	-3.614137000	-3.114004000	-3.358798000
N	0.694519000	-5.861464000	-1.611187000
O	-0.005343000	-6.654604000	-1.018769000
O	1.802901000	-6.053548000	-2.109757000
N	0.955441000	-3.202059000	0.189596000
O	1.228441000	-4.185153000	0.865609000
O	0.526806000	-2.125450000	0.567643000

$1_{\text{O}}^{-}(\text{c}) / \text{BP86-D3(BJ)/Def2-TZVP}$

C	-1.877947000	1.954444000	2.188513000
O	-2.518095000	0.730027000	2.416633000
O	-0.220156000	0.809460000	1.075786000
C	-0.361712000	1.762232000	2.061470000
O	0.741074000	-0.078853000	-2.188595000
C	0.267676000	0.752102000	-1.224814000
C	0.881278000	0.865170000	0.191694000
O	1.453081000	-2.431182000	-2.182410000
C	2.612273000	-1.626173000	-2.532665000
C	2.075706000	-0.168531000	-2.741323000
C	-3.178341000	0.172439000	1.334979000
C	-3.216968000	-1.350972000	1.425158000
O	-1.994323000	-1.855010000	1.017425000
C	-1.999774000	-3.048496000	0.288921000
C	-1.133011000	-2.887196000	-0.974569000

O	-0.823800000	-4.144286000	-1.433444000
C	0.092889000	-4.295607000	-2.505146000
C	1.520550000	-3.808195000	-2.264982000
C	3.035514000	0.941025000	-2.253236000
C	3.365839000	-2.087627000	-3.830590000
O	2.588859000	1.929945000	-1.641078000
N	4.312851000	0.740147000	-2.578391000
C	5.352076000	1.687808000	-2.232064000
O	4.397792000	-1.401167000	-4.093619000
O	2.895368000	-3.046930000	-4.477889000
H	-2.216073000	2.443446000	1.264010000
H	0.139893000	2.716996000	1.846673000
H	-0.764527000	0.397055000	-1.062779000
H	1.519872000	1.740564000	0.323853000
H	3.304731000	-1.655762000	-1.679582000
H	1.918339000	-0.005641000	-3.818828000
H	-2.723451000	0.424388000	0.365327000
H	-4.068564000	-1.723710000	0.837241000
H	-3.012159000	-3.404452000	0.051408000
H	-0.279482000	-2.216374000	-0.798155000
H	-0.268920000	-3.790066000	-3.410942000
H	2.167128000	-4.131993000	-3.106969000
H	4.514396000	-0.127106000	-3.176701000
H	6.176730000	1.171037000	-1.720278000
H	4.933800000	2.453135000	-1.567473000
H	5.754411000	2.176763000	-3.133325000
N	0.005251000	2.222110000	-1.733944000
O	-0.047703000	2.404005000	-2.934137000
O	-0.250751000	3.055468000	-0.854629000
N	1.762188000	-0.372127000	0.499820000
O	1.170274000	-1.428452000	0.675748000
O	2.972416000	-0.191030000	0.541610000
N	0.296607000	1.252311000	3.391144000
O	1.246995000	0.496915000	3.259426000
O	-0.161450000	1.693451000	4.439275000
N	-2.252399000	2.969695000	3.294904000
O	-3.042604000	2.640471000	4.154068000
O	-1.711224000	4.064967000	3.143834000
N	-4.638785000	0.750584000	1.199298000
O	-5.416690000	0.106332000	0.503831000

O	-4.839486000	1.836070000	1.720004000
N	-3.552237000	-1.779799000	2.894259000
O	-4.527916000	-1.214223000	3.377957000
O	-2.863071000	-2.647797000	3.399645000
N	-1.390849000	-4.187313000	1.171638000
O	-2.106739000	-5.171686000	1.321734000
O	-0.283915000	-3.984045000	1.635833000
N	-2.045108000	-2.113608000	-2.009808000
O	-2.342553000	-2.683712000	-3.046163000
O	-2.403589000	-0.978228000	-1.681188000
N	0.039760000	-5.795665000	-2.875308000
O	0.838255000	-6.126924000	-3.745748000
O	-0.808883000	-6.495124000	-2.348930000
N	2.120746000	-4.443309000	-0.986324000
O	2.942656000	-3.780788000	-0.365873000
O	1.782189000	-5.603786000	-0.743404000

2_{Fe}⁺(a)···Li⁺ / BP86–D3(BJ)/Def2–TZVP

Fe	-1.992927000	-0.415984000	1.647497000
C	-3.367747000	1.081886000	1.943879000
C	-3.774192000	0.261126000	0.846514000
C	-2.766971000	0.333358000	-0.168968000
C	-1.770780000	1.264101000	0.278767000
C	-2.093093000	1.658111000	1.623926000
C	-2.215393000	-2.442150000	1.942221000
C	-2.301842000	-1.766371000	3.197075000
C	-1.064111000	-1.086327000	3.432083000
C	-0.191697000	-1.402474000	2.344828000
C	-0.918720000	-2.176788000	1.379563000
O	1.092028000	-1.011387000	2.161043000
O	3.595735000	-0.017362000	1.894214000
O	4.062764000	-0.315391000	-0.654288000
O	1.537940000	-0.090000000	-1.382963000
O	-0.644993000	1.660160000	-0.323145000
C	4.976546000	-0.252657000	1.519253000
C	5.126396000	0.284059000	0.114817000
C	3.836095000	0.295399000	-1.935911000
C	2.525422000	-0.257433000	-2.444083000
C	0.171121000	-0.100123000	-1.838233000
C	-0.459596000	1.274502000	-1.713735000

C	1.747411000	-0.389052000	3.320440000
C	3.232578000	-0.585036000	3.157168000
H	-3.919709000	1.240668000	2.865870000
H	-4.684439000	-0.328951000	0.787479000
H	-2.795867000	-0.196352000	-1.115523000
H	-1.517662000	2.350063000	2.231555000
H	-2.987904000	-3.055656000	1.487681000
H	-3.161455000	-1.751919000	3.861136000
H	-0.842812000	-0.462805000	4.292297000
H	-0.517720000	-2.588409000	0.457753000
H	5.182090000	-1.335648000	1.557480000
H	5.656251000	0.269724000	2.209801000
H	5.015626000	1.381818000	0.098550000
H	6.110538000	0.016329000	-0.300217000
H	4.649166000	0.054349000	-2.639697000
H	3.781433000	1.391565000	-1.815746000
H	2.214751000	0.295030000	-3.343242000
H	2.605017000	-1.328829000	-2.686981000
H	-0.378481000	-0.838922000	-1.235760000
H	0.122571000	-0.423456000	-2.888752000
H	0.196571000	2.048290000	-2.130063000
H	-1.425974000	1.312106000	-2.237675000
H	1.404149000	-0.880453000	4.240046000
H	1.475051000	0.676641000	3.334270000
H	3.756665000	-0.078109000	3.985093000
H	3.492051000	-1.657817000	3.180299000
Li	2.388683000	-0.378123000	0.374123000

2_{Fe}(a)···Li⁺ / BP86–D3(BJ)/Def2–TZVP

Fe	-0.895441000	-0.715458000	1.648804000
C	-2.646909000	-0.522189000	0.641835000
C	-1.759715000	-1.415533000	-0.048475000
C	-0.550592000	-0.720821000	-0.369870000
C	-0.700668000	0.615652000	0.163872000
C	-1.984387000	0.745734000	0.777431000
C	-2.350281000	-2.487812000	3.495835000
C	-2.657227000	-1.227434000	3.952786000
C	-1.494576000	-0.367638000	3.775483000
C	-0.420485000	-1.258040000	3.450966000
C	-0.974711000	-2.500216000	3.017019000

O	0.794656000	-0.830003000	2.864069000
O	3.068424000	0.125732000	1.574274000
O	3.001970000	-0.779631000	-0.961048000
O	1.913902000	1.386758000	-1.978774000
O	0.288009000	1.607984000	0.151643000
C	3.431552000	-1.253251000	1.312463000
C	4.011772000	-1.302407000	-0.080784000
C	3.476126000	-0.366257000	-2.255023000
C	2.328599000	0.372854000	-2.908417000
C	0.611747000	1.940831000	-2.239693000
C	0.153830000	2.568886000	-0.939042000
C	1.352969000	0.434989000	3.311135000
C	2.828162000	0.416007000	2.970490000
H	-3.618550000	-0.783263000	1.049129000
H	-1.960991000	-2.461696000	-0.259855000
H	0.320490000	-1.130269000	-0.876383000
H	-2.360967000	1.631499000	1.279874000
H	-3.005053000	-3.355264000	3.503280000
H	-3.598558000	-0.906883000	4.390829000
H	-1.401055000	0.650894000	4.141222000
H	-0.407393000	-3.374153000	2.710626000
H	2.539227000	-1.892900000	1.400211000
H	4.186877000	-1.587000000	2.040868000
H	4.918215000	-0.675998000	-0.146514000
H	4.269783000	-2.338770000	-0.354255000
H	3.771488000	-1.236956000	-2.862648000
H	4.350980000	0.295949000	-2.131173000
H	2.650130000	0.817943000	-3.864186000
H	1.484997000	-0.312499000	-3.102464000
H	-0.076466000	1.134477000	-2.545770000
H	0.658136000	2.694276000	-3.043515000
H	0.796529000	3.412665000	-0.654947000
H	-0.888216000	2.910671000	-1.008909000
H	1.221395000	0.535173000	4.398775000
H	0.824758000	1.254147000	2.801285000
H	3.258604000	1.407215000	3.175958000
H	3.358945000	-0.327123000	3.583299000
Li	2.040551000	0.704410000	-0.039984000

$2_{\text{Fe}^+}(\text{a}) \cdots \text{Na}^+ / \text{BP86-D3(BJ)/Def2-TZVP}$

Fe	-2.082308000	-0.528646000	1.913131000
C	-3.115815000	1.282416000	1.843972000
C	-3.793007000	0.357322000	0.993539000
C	-2.882730000	-0.090220000	-0.005516000
C	-1.637745000	0.589828000	0.206502000
C	-1.767581000	1.431408000	1.367765000
C	-2.516682000	-2.444954000	2.518065000
C	-2.518259000	-1.565185000	3.646868000
C	-1.208370000	-0.997673000	3.776653000
C	-0.384913000	-1.585656000	2.759763000
C	-1.206605000	-2.421349000	1.933816000
O	0.908526000	-1.352241000	2.483906000
O	3.417815000	-0.169555000	1.934813000
O	4.025546000	-0.066161000	-0.749782000
O	1.753006000	0.653574000	-2.076409000
O	-0.496939000	0.430862000	-0.529126000
C	4.774584000	-0.407198000	1.484821000
C	5.004068000	0.364146000	0.208370000
C	4.130062000	0.609367000	-2.015121000
C	2.913495000	0.242040000	-2.830824000
C	0.511982000	0.383184000	-2.729000000
C	-0.587132000	0.988865000	-1.893826000
C	1.686409000	-0.648681000	3.508847000
C	3.145101000	-0.823696000	3.176720000
H	-3.546527000	1.788962000	2.703554000
H	-4.815802000	0.011262000	1.118336000
H	-3.085256000	-0.831066000	-0.774759000
H	-1.007705000	2.097035000	1.767089000
H	-3.358459000	-3.028878000	2.156579000
H	-3.363002000	-1.353109000	4.296333000
H	-0.900166000	-0.278348000	4.529196000
H	-0.867103000	-2.984033000	1.069188000
H	4.914660000	-1.489130000	1.319149000
H	5.489698000	-0.069357000	2.252746000
H	4.906607000	1.451225000	0.381163000
H	6.025460000	0.160744000	-0.155994000
H	5.045566000	0.299217000	-2.545905000
H	4.168504000	1.701171000	-1.853723000
H	2.941454000	0.763116000	-3.801774000

H	2.872813000	-0.846377000	-3.013663000
H	0.366746000	-0.706386000	-2.850476000
H	0.481089000	0.846232000	-3.731261000
H	-0.477283000	2.079909000	-1.812394000
H	-1.569463000	0.745666000	-2.321969000
H	1.468270000	-1.090554000	4.491075000
H	1.396011000	0.413791000	3.505110000
H	3.745625000	-0.380143000	3.990721000
H	3.394378000	-1.897511000	3.109031000
Na	1.861927000	-0.099955000	0.156439000

2_{Fe}(a)···Na⁺ / BP86–D3(BJ)/Def2–TZVP

Fe	-2.131444000	-0.435759000	1.913521000
C	-3.589646000	0.824609000	1.219215000
C	-3.807617000	-0.508360000	0.734122000
C	-2.652826000	-0.914428000	-0.007794000
C	-1.719208000	0.174120000	0.038766000
C	-2.294697000	1.257458000	0.786656000
C	-2.525345000	-1.726387000	3.456854000
C	-2.339653000	-0.391960000	3.951089000
C	-1.036447000	0.057010000	3.562942000
C	-0.428358000	-1.012856000	2.821226000
C	-1.337256000	-2.121319000	2.762486000
O	0.873618000	-1.024122000	2.330780000
O	3.545930000	-0.570981000	1.891432000
O	4.020654000	0.121054000	-0.703914000
O	1.766041000	1.000283000	-1.961490000
O	-0.499940000	0.205372000	-0.630587000
C	4.832671000	-0.815329000	1.311266000
C	5.070185000	0.240308000	0.261158000
C	4.131937000	1.062344000	-1.775633000
C	2.973789000	0.814799000	-2.708979000
C	0.597239000	0.662398000	-2.715096000
C	-0.608283000	0.963108000	-1.865114000
C	1.830289000	-1.208539000	3.408295000
C	3.154655000	-1.598193000	2.807916000
H	-4.277590000	1.395874000	1.835259000
H	-4.687723000	-1.115604000	0.923290000
H	-2.491827000	-1.869728000	-0.498295000
H	-1.825745000	2.214681000	0.995306000

H	-3.424859000	-2.324261000	3.568754000
H	-3.074786000	0.189837000	4.499017000
H	-0.593294000	1.025996000	3.773612000
H	-1.154344000	-3.067633000	2.262470000
H	4.852638000	-1.820898000	0.852651000
H	5.620329000	-0.766431000	2.083618000
H	5.058238000	1.249737000	0.712013000
H	6.055091000	0.080800000	-0.212395000
H	5.084598000	0.925406000	-2.317299000
H	4.100018000	2.093994000	-1.379355000
H	3.014277000	1.518629000	-3.558847000
H	3.015872000	-0.216483000	-3.104736000
H	0.625352000	-0.408016000	-2.991660000
H	0.546143000	1.259616000	-3.643204000
H	-0.665756000	2.037256000	-1.626315000
H	-1.525099000	0.666684000	-2.397880000
H	1.475963000	-2.005124000	4.080596000
H	1.916201000	-0.270744000	3.980329000
H	3.901956000	-1.705775000	3.614574000
H	3.075201000	-2.564634000	2.276297000
Na	1.713410000	-0.042528000	0.294820000

2_{Fe}⁺(a)---K⁺ / BP86-D3(BJ)/Def2-TZVP

Fe	-2.159571000	-0.639365000	1.845515000
C	-3.727001000	0.493521000	1.145805000
C	-3.830872000	-0.859419000	0.689068000
C	-2.676630000	-1.151360000	-0.111824000
C	-1.920909000	0.060296000	-0.225020000
C	-2.514786000	1.053802000	0.620682000
C	-2.580267000	-1.945898000	3.360784000
C	-2.455753000	-0.618146000	3.881381000
C	-1.119430000	-0.160108000	3.629810000
C	-0.406239000	-1.246187000	3.025226000
C	-1.325239000	-2.314858000	2.770264000
O	0.881680000	-1.294071000	2.638978000
O	3.489693000	-0.599850000	1.689182000
O	4.170516000	-0.387147000	-0.976243000
O	1.839766000	0.803171000	-1.861867000
O	-0.790136000	0.138835000	-0.949026000
C	4.808714000	-1.000997000	1.258689000

C	5.169131000	-0.188264000	0.036612000
C	4.222072000	0.622746000	-1.996017000
C	2.932973000	0.601990000	-2.784469000
C	0.656590000	1.330841000	-2.458820000
C	-0.379316000	1.484105000	-1.374141000
C	1.807420000	-0.399873000	3.348887000
C	3.212738000	-0.865127000	3.062967000
H	-4.441035000	1.015405000	1.776305000
H	-4.638602000	-1.552221000	0.906194000
H	-2.463629000	-2.082191000	-0.629021000
H	-2.159342000	2.066576000	0.783303000
H	-3.465895000	-2.573349000	3.401357000
H	-3.231966000	-0.049815000	4.385505000
H	-0.713960000	0.806788000	3.911477000
H	-1.079637000	-3.267728000	2.310914000
H	4.820125000	-2.085595000	1.048141000
H	5.549691000	-0.799495000	2.049440000
H	5.206523000	0.881681000	0.305044000
H	6.164904000	-0.492146000	-0.330205000
H	5.074586000	0.450133000	-2.675557000
H	4.345621000	1.611877000	-1.522014000
H	2.961446000	1.413749000	-3.529468000
H	2.796202000	-0.352731000	-3.323313000
H	0.279698000	0.669275000	-3.259769000
H	0.851226000	2.325990000	-2.897749000
H	0.039140000	2.021454000	-0.509547000
H	-1.262498000	2.014293000	-1.756697000
H	1.593634000	-0.459718000	4.425009000
H	1.656249000	0.629763000	2.990818000
H	3.904515000	-0.303795000	3.716648000
H	3.316636000	-1.940539000	3.295247000
K	1.751742000	-1.331026000	-0.226743000

2_{Fe}^{+(a)}...K⁺ / ZORA-BP86-D3(BJ)/Def2-TZVP

Fe	-2.160352000	-0.639430000	1.846714000
C	-3.721605000	0.492382000	1.149425000
C	-3.826941000	-0.860700000	0.694824000
C	-2.671899000	-1.154672000	-0.105075000
C	-1.916158000	0.055907000	-0.220876000
C	-2.508196000	1.049694000	0.623993000

C	-2.583230000	-1.940137000	3.358011000
C	-2.456816000	-0.611868000	3.876103000
C	-1.120112000	-0.156356000	3.622657000
C	-0.408187000	-1.244319000	3.021509000
C	-1.328602000	-2.311407000	2.767869000
O	0.879835000	-1.295553000	2.635230000
O	3.486264000	-0.600937000	1.687854000
O	4.169098000	-0.384569000	-0.976248000
O	1.840948000	0.805805000	-1.859870000
O	-0.787077000	0.133177000	-0.948442000
C	4.806591000	-1.000532000	1.257534000
C	5.166950000	-0.185009000	0.037925000
C	4.222346000	0.626363000	-1.995505000
C	2.934037000	0.605631000	-2.784092000
C	0.655893000	1.328484000	-2.459253000
C	-0.379770000	1.480309000	-1.375028000
C	1.806606000	-0.403904000	3.349141000
C	3.210548000	-0.869823000	3.061894000
H	-4.434165000	1.015470000	1.780661000
H	-4.635032000	-1.552500000	0.914023000
H	-2.458923000	-2.087006000	-0.619531000
H	-2.149699000	2.061236000	0.787738000
H	-3.470082000	-2.565922000	3.398928000
H	-3.232758000	-0.041030000	4.377903000
H	-0.714117000	0.811400000	3.900712000
H	-1.083939000	-3.265635000	2.310794000
H	4.818628000	-2.084427000	1.044100000
H	5.546647000	-0.799803000	2.049272000
H	5.201944000	0.884538000	0.308038000
H	6.163503000	-0.487066000	-0.328221000
H	5.075399000	0.453980000	-2.674408000
H	4.345626000	1.615245000	-1.520957000
H	2.961377000	1.417960000	-3.528432000
H	2.797641000	-0.348996000	-3.323052000
H	0.282228000	0.664935000	-3.259849000
H	0.847587000	2.324225000	-2.898166000
H	0.036814000	2.019380000	-0.510808000
H	-1.264848000	2.006664000	-1.758521000
H	1.591814000	-0.467513000	4.424793000
H	1.656752000	0.626678000	2.993496000

H	3.902815000	-0.309721000	3.716082000
H	3.314667000	-1.945713000	3.291396000
K	1.750466000	-1.329644000	-0.230543000

2_{Fe}(a)···K⁺ / BP86–D3(BJ)/Def2–TZVP

Fe	-2.065127000	-0.403713000	1.901143000
C	-3.481364000	0.909178000	1.225900000
C	-3.810318000	-0.431158000	0.833931000
C	-2.740173000	-0.945441000	0.034506000
C	-1.753537000	0.087992000	-0.066509000
C	-2.201227000	1.236515000	0.674359000
C	-2.564115000	-1.568942000	3.505906000
C	-2.232999000	-0.239852000	3.932806000
C	-0.890281000	0.041823000	3.523439000
C	-0.399266000	-1.129952000	2.849445000
C	-1.430596000	-2.123905000	2.831073000
O	0.886582000	-1.306476000	2.363884000
O	3.590758000	-0.591034000	2.041295000
O	3.955521000	0.287525000	-0.610248000
O	1.687227000	1.126635000	-2.052916000
O	-0.595358000	0.014151000	-0.823754000
C	4.829491000	-0.759075000	1.340265000
C	5.002845000	0.379202000	0.360177000
C	4.055130000	1.237280000	-1.675712000
C	2.963179000	0.930338000	-2.675448000
C	0.611273000	0.573184000	-2.820819000
C	-0.683246000	0.754358000	-2.067114000
C	1.862646000	-1.536312000	3.410599000
C	3.206162000	-1.767096000	2.763985000
H	-4.087401000	1.554459000	1.854641000
H	-4.706757000	-0.972587000	1.120888000
H	-2.670558000	-1.932258000	-0.412581000
H	-1.681102000	2.185801000	0.774196000
H	-3.523398000	-2.058154000	3.645524000
H	-2.895883000	0.444085000	4.454228000
H	-0.338685000	0.959146000	3.712788000
H	-1.352760000	-3.107519000	2.378332000
H	4.819767000	-1.717680000	0.790875000
H	5.675781000	-0.771620000	2.050359000
H	4.965779000	1.355414000	0.880832000

H	5.991048000	0.290156000	-0.125863000
H	5.036615000	1.157159000	-2.176668000
H	3.953741000	2.268736000	-1.286854000
H	3.068080000	1.589655000	-3.555735000
H	3.056846000	-0.118199000	-3.010905000
H	0.798866000	-0.500759000	-3.002989000
H	0.530026000	1.082260000	-3.798481000
H	-0.869307000	1.819680000	-1.851010000
H	-1.519817000	0.367468000	-2.671219000
H	1.576830000	-2.424619000	3.996710000
H	1.893911000	-0.664643000	4.085477000
H	3.946596000	-1.998893000	3.551195000
H	3.153623000	-2.627681000	2.072296000
K	1.535511000	0.580614000	0.635469000

2_{Fe}(a)---K⁺ / ZORA-BP86-D3(BJ)/Def2-TZVP

Fe	-2.065114000	-0.405625000	1.898512000
C	-3.480737000	0.903804000	1.233709000
C	-3.806254000	-0.435911000	0.836832000
C	-2.734347000	-0.945190000	0.036680000
C	-1.749289000	0.090149000	-0.059382000
C	-2.200423000	1.235505000	0.684634000
C	-2.563405000	-1.573293000	3.494239000
C	-2.235011000	-0.244645000	3.924339000
C	-0.893141000	0.040110000	3.514065000
C	-0.399834000	-1.129434000	2.838081000
C	-1.429043000	-2.125214000	2.817735000
O	0.888438000	-1.303155000	2.355913000
O	3.592227000	-0.584508000	2.045209000
O	3.956195000	0.280277000	-0.610790000
O	1.687908000	1.127598000	-2.052432000
O	-0.589684000	0.020692000	-0.816701000
C	4.830670000	-0.756589000	1.344005000
C	5.003476000	0.377686000	0.359880000
C	4.057391000	1.224723000	-1.681116000
C	2.961515000	0.918719000	-2.676514000
C	0.606726000	0.581327000	-2.818917000
C	-0.682875000	0.765025000	-2.057910000
C	1.859884000	-1.526899000	3.409490000
C	3.205771000	-1.759521000	2.769441000

H	-4.087460000	1.544698000	1.866313000
H	-4.700648000	-0.981166000	1.122844000
H	-2.663248000	-1.931454000	-0.411562000
H	-1.681044000	2.184435000	0.791556000
H	-3.521747000	-2.064748000	3.632860000
H	-2.899422000	0.437059000	4.446753000
H	-0.343499000	0.959489000	3.698924000
H	-1.351017000	-3.107765000	2.362619000
H	4.820005000	-1.717802000	0.799268000
H	5.677372000	-0.766030000	2.053642000
H	4.964012000	1.355436000	0.877324000
H	5.991846000	0.287987000	-0.125532000
H	5.036777000	1.137101000	-2.185083000
H	3.961876000	2.258791000	-1.297849000
H	3.069740000	1.572538000	-3.560425000
H	3.046999000	-0.132511000	-3.005527000
H	0.788958000	-0.492712000	-3.005371000
H	0.524388000	1.094849000	-3.794121000
H	-0.863885000	1.830429000	-1.837898000
H	-1.524512000	0.382468000	-2.657578000
H	1.571374000	-2.412547000	3.998344000
H	1.885313000	-0.652476000	4.081008000
H	3.944724000	-1.989886000	3.558260000
H	3.152939000	-2.620535000	2.078471000
K	1.539675000	0.583963000	0.635457000

2_{Fe}⁺(b)---Na⁺ / BP86-D3(BJ)/Def2-TZVP

Fe	-1.852139000	-0.112533000	2.015835000
C	-3.521626000	1.172480000	1.759404000
C	-3.670230000	0.005603000	0.921336000
C	-2.494721000	-0.121898000	0.094733000
C	-1.655999000	1.035200000	0.371520000
C	-2.354727000	1.884995000	1.304260000
C	-1.712837000	-2.121763000	2.495747000
C	-2.087504000	-1.446769000	3.720191000
C	-1.126000000	-0.416481000	3.978929000
C	-0.113029000	-0.491955000	2.936158000
C	-0.455291000	-1.563913000	2.029616000
O	0.991878000	0.320693000	2.861703000
O	3.452743000	-0.641554000	1.867915000

O	3.536992000	-0.782865000	-0.882344000
O	1.575329000	0.809677000	-1.992335000
O	-0.453137000	1.367489000	-0.200860000
C	4.351638000	-1.550557000	1.212591000
C	4.737191000	-0.946177000	-0.115744000
C	3.753263000	-0.151892000	-2.151265000
C	2.410984000	-0.012062000	-2.826645000
C	0.242831000	0.931191000	-2.490942000
C	-0.503353000	1.873891000	-1.576791000
C	2.103613000	-0.063313000	3.734049000
C	2.962082000	-1.139049000	3.110555000
H	3.852898000	-2.525584000	1.061417000
H	5.253280000	-1.710057000	1.828238000
H	5.228450000	0.032367000	0.032935000
H	5.443779000	-1.615801000	-0.636122000
H	4.420919000	-0.763729000	-2.782496000
H	4.220595000	0.838937000	-2.006590000
H	2.537343000	0.454205000	-3.818523000
H	1.942820000	-1.004130000	-2.960280000
H	-0.242605000	-0.062171000	-2.511655000
H	0.242386000	1.344807000	-3.516054000
H	-0.020565000	2.860917000	-1.564886000
H	-1.548867000	1.984817000	-1.896028000
H	1.715487000	-0.399779000	4.706875000
H	2.681247000	0.859495000	3.869401000
H	3.794815000	-1.374600000	3.798467000
H	2.381820000	-2.068430000	2.952034000
Na	1.679606000	0.129255000	0.363847000
N	-1.898567000	3.072583000	1.789472000
H	-2.559320000	3.735646000	2.181942000
H	-1.088096000	3.483495000	1.336493000
N	-4.478904000	1.659508000	2.646633000
H	-4.105674000	2.276239000	3.367589000
H	-5.038008000	0.934424000	3.094753000
N	-4.723336000	-0.890785000	0.969093000
H	-5.598508000	-0.518133000	1.331555000
H	-4.877420000	-1.404883000	0.103159000
N	-2.176415000	-1.195918000	-0.767512000
H	-2.487824000	-1.068413000	-1.731869000
H	-2.527154000	-2.085647000	-0.393309000

N	-1.183596000	0.490856000	5.032019000
H	-0.470691000	1.216080000	4.998226000
H	-1.262113000	0.088565000	5.965734000
N	0.290602000	-1.890934000	0.864247000
H	-0.339474000	-1.930933000	0.046802000
H	0.770433000	-2.790312000	0.951002000
N	-3.243606000	-1.683050000	4.429174000
H	-3.368496000	-1.173322000	5.297952000
H	-3.573284000	-2.643648000	4.472502000
N	-2.443163000	-3.101251000	1.800048000
H	-3.436949000	-3.107426000	2.032887000
H	-2.052995000	-4.042724000	1.850328000

2_{Fe}(b)···Na⁺ / BP86–D3(BJ)/Def2–TZVP

Fe	-1.861404000	-0.556940000	1.790980000
C	-2.928706000	0.986959000	1.028387000
C	-3.656920000	-0.264755000	0.864442000
C	-2.843907000	-1.151070000	0.075208000
C	-1.603154000	-0.475058000	-0.201681000
C	-1.677288000	0.860430000	0.333536000
C	-2.480085000	-1.519695000	3.531786000
C	-1.906057000	-0.234828000	3.818438000
C	-0.564792000	-0.212300000	3.271914000
C	-0.345076000	-1.502265000	2.642745000
C	-1.532280000	-2.308250000	2.791694000
O	0.847281000	-1.899185000	2.055237000
O	3.256059000	-0.531121000	2.134513000
O	3.294442000	1.021451000	-0.131390000
O	1.208551000	1.013140000	-1.956711000
O	-0.548008000	-0.957922000	-0.964083000
C	4.493775000	-0.093015000	1.571768000
C	4.251666000	1.244061000	0.908712000
C	3.143889000	2.096693000	-1.062958000
C	2.501086000	1.519399000	-2.304364000
C	0.789863000	-0.080562000	-2.777115000
C	-0.591907000	-0.501890000	-2.341116000
C	1.873374000	-2.248630000	3.017156000
C	3.219894000	-1.932057000	2.413621000
H	4.844055000	-0.818159000	0.814970000
H	5.268939000	0.000963000	2.353717000

H	3.869798000	1.982610000	1.637584000
H	5.198816000	1.625729000	0.488465000
H	4.128123000	2.521677000	-1.327590000
H	2.524405000	2.902599000	-0.627864000
H	2.417166000	2.292362000	-3.089157000
H	3.134270000	0.699738000	-2.685944000
H	1.502752000	-0.919043000	-2.669869000
H	0.757371000	0.211929000	-3.843057000
H	-1.297175000	0.339741000	-2.424205000
H	-0.948075000	-1.319560000	-2.988955000
H	1.809610000	-3.321508000	3.261968000
H	1.719552000	-1.668714000	3.940018000
H	4.014661000	-2.215314000	3.127969000
H	3.374030000	-2.505392000	1.480227000
Na	1.176425000	0.207919000	0.828716000
N	0.393988000	0.843244000	3.269917000
H	1.009728000	0.836640000	4.087520000
H	-0.066347000	1.754144000	3.215914000
N	-2.536515000	0.857844000	4.458819000
H	-1.967539000	1.264082000	5.202669000
H	-3.453462000	0.619756000	4.834422000
N	-3.789903000	-1.953012000	3.823528000
H	-4.078952000	-1.735560000	4.778588000
H	-3.841314000	-2.968026000	3.687439000
N	-1.817445000	-3.607534000	2.325614000
H	-0.964020000	-4.138782000	2.153762000
H	-2.348573000	-3.560194000	1.437040000
N	-0.672716000	1.856272000	0.248828000
H	-1.044521000	2.714439000	0.668622000
H	-0.385532000	2.037418000	-0.717414000
N	-3.273690000	2.163892000	1.738551000
H	-3.240569000	2.017549000	2.757784000
H	-4.175283000	2.555147000	1.466082000
N	-4.934359000	-0.614080000	1.345894000
H	-5.500914000	0.213929000	1.531470000
H	-4.867772000	-1.163220000	2.221568000
N	-3.183032000	-2.479375000	-0.231958000
H	-2.759828000	-2.815633000	-1.095312000
H	-4.199158000	-2.593867000	-0.254916000

$2_{\text{Fe}^+}(\text{c})\cdots\text{Na}^+ / \text{BP86-D3(BJ)/Def2-TZVP}$

Fe	-1.793665000	-0.510128000	1.907505000
C	-2.731836000	0.933481000	0.906644000
C	-3.764957000	0.714948000	-0.091330000
C	-3.288575000	1.017130000	-1.340941000
C	-1.924634000	1.536576000	-1.222642000
C	-1.621756000	1.551037000	0.149898000
C	-2.234024000	-2.027081000	3.208723000
C	-2.098324000	-1.718310000	4.621448000
C	-0.757639000	-1.631588000	4.990631000
C	0.066365000	-1.952038000	3.853152000
C	-0.847292000	-2.238788000	2.773683000
O	1.338390000	-1.903291000	3.590237000
O	3.374288000	-0.368878000	2.258944000
O	3.572697000	0.182813000	-0.525718000
O	1.083610000	-0.105180000	-1.796120000
O	-1.045585000	1.814499000	-2.151490000
C	4.631059000	-0.027341000	1.616072000
C	4.368577000	0.888636000	0.444891000
C	3.247249000	0.974419000	-1.680256000
C	2.291659000	0.191349000	-2.550191000
C	-0.056835000	-0.389933000	-2.613210000
C	-0.716768000	0.847072000	-3.218327000
C	2.343734000	-1.097976000	4.328335000
C	3.590665000	-1.084318000	3.484764000
H	5.141538000	-0.948880000	1.287296000
H	5.281691000	0.496235000	2.335729000
H	3.835913000	1.799369000	0.770603000
H	5.334624000	1.184831000	0.002588000
H	4.159723000	1.196238000	-2.259552000
H	2.789957000	1.926839000	-1.362786000
H	2.055649000	0.800460000	-3.435744000
H	2.740500000	-0.757710000	-2.886963000
H	-0.770446000	-0.922834000	-1.966504000
H	0.203704000	-1.067547000	-3.445533000
H	-0.054007000	1.424869000	-3.869763000
H	-1.613747000	0.560776000	-3.782689000
H	2.525841000	-1.578293000	5.295718000
H	1.917335000	-0.095604000	4.469854000
H	4.371281000	-0.582710000	4.083955000

H	3.931089000	-2.114759000	3.281216000
Na	1.862418000	-0.901316000	0.439365000
N	-0.320305000	1.452692000	0.624460000
O	0.632330000	2.059825000	0.190657000
O	-0.152733000	0.506389000	1.557817000
N	-3.077567000	1.576070000	2.234132000
O	-3.783443000	2.509215000	2.445623000
O	-2.422160000	0.898054000	3.118812000
N	-5.072341000	0.181733000	0.269411000
O	-5.154001000	-0.211755000	1.442820000
O	-5.931492000	0.150461000	-0.598065000
N	-3.977750000	0.828026000	-2.628320000
O	-4.483778000	1.829167000	-3.104671000
O	-3.918311000	-0.305093000	-3.096136000
N	-0.302012000	-1.371073000	6.357245000
O	0.801584000	-1.838090000	6.650720000
O	-1.065284000	-0.750397000	7.084114000
N	-0.483242000	-2.463426000	1.446035000
O	-1.311006000	-1.853136000	0.611618000
O	0.557399000	-2.980521000	1.074007000
N	-3.240228000	-1.559355000	5.531843000
O	-3.800314000	-0.477150000	5.485211000
O	-3.497654000	-2.535911000	6.216926000
N	-3.370984000	-2.935955000	2.757432000
O	-4.440500000	-2.725859000	3.303375000
O	-3.096865000	-3.752024000	1.890560000

2_{Fe}(c)···Na⁺ / BP86–D3(BJ)/Def2–TZVP

Fe	-1.580428000	0.411119000	1.880918000
C	-3.066535000	1.562200000	1.187543000
C	-3.392209000	0.180184000	1.021068000
C	-2.396485000	-0.424169000	0.188817000
C	-1.415693000	0.581318000	-0.141750000
C	-1.839128000	1.822192000	0.472536000
C	-2.357967000	-2.726644000	4.012231000
C	-2.584794000	-1.490957000	4.642804000
C	-1.728977000	-0.538479000	4.046940000
C	-0.981196000	-1.217673000	2.983736000
C	-1.367707000	-2.585325000	3.021602000
O	0.095286000	-0.657720000	2.323013000

O	2.915479000	-0.002168000	1.357997000
O	4.062868000	1.520358000	-0.759685000
O	1.949155000	0.696308000	-2.367616000
O	-0.271123000	0.409456000	-0.820792000
C	4.090331000	-0.488616000	0.670064000
C	4.857075000	0.694508000	0.106038000
C	4.229434000	1.326864000	-2.175546000
C	3.273854000	0.289041000	-2.736734000
C	0.927865000	-0.212069000	-2.788975000
C	-0.388284000	0.321424000	-2.294049000
C	1.308248000	-0.331210000	3.124659000
C	2.514008000	-0.884421000	2.414224000
H	3.784288000	-1.206065000	-0.110079000
H	4.746772000	-1.018004000	1.381550000
H	5.183002000	1.344237000	0.931605000
H	5.753831000	0.330076000	-0.421007000
H	5.269665000	1.049284000	-2.408407000
H	4.021987000	2.304901000	-2.632194000
H	3.374470000	0.249136000	-3.835898000
H	3.480322000	-0.720233000	-2.336642000
H	1.111734000	-1.219937000	-2.377067000
H	0.891594000	-0.282336000	-3.890611000
H	-0.587589000	1.335368000	-2.669790000
H	-1.204842000	-0.363360000	-2.548675000
H	1.190257000	-0.811414000	4.104012000
H	1.349535000	0.758774000	3.244466000
H	3.332652000	-0.966687000	3.152677000
H	2.287239000	-1.890950000	2.023325000
Na	1.793996000	1.529645000	-0.114248000
N	-1.424296000	0.783893000	4.433247000
O	-1.062005000	1.510571000	3.391027000
O	-1.463489000	1.225014000	5.551079000
N	-3.680138000	-1.192596000	5.547676000
O	-3.997377000	-0.007287000	5.658672000
O	-4.192133000	-2.154263000	6.119374000
N	-3.113308000	-3.964733000	4.281455000
O	-4.133300000	-4.117756000	3.626177000
O	-2.629150000	-4.701762000	5.126235000
N	-0.793674000	-3.632795000	2.217078000
O	0.083391000	-3.287888000	1.403721000

O	-1.204302000	-4.775726000	2.394587000
N	-1.173183000	3.092540000	0.243246000
O	-1.866811000	4.064622000	0.006614000
O	0.076008000	3.077851000	0.268603000
N	-3.843667000	2.529178000	1.986490000
O	-5.041998000	2.290729000	2.092545000
O	-3.210206000	3.462123000	2.468066000
N	-4.627631000	-0.481777000	1.507933000
O	-4.693879000	-0.738875000	2.699718000
O	-5.455037000	-0.686313000	0.634114000
N	-2.358639000	-1.836016000	-0.172131000
O	-1.666977000	-2.149890000	-1.141835000
O	-3.022834000	-2.591571000	0.536418000

2_{Fe}⁺(d)···Na⁺ / BP86–D3(BJ)/Def2–TZVP

Fe	-2.039523000	-0.502108000	1.903070000
C	-3.410086000	1.010749000	1.685943000
C	-3.786092000	-0.095897000	0.861769000
C	-2.732373000	-0.336693000	-0.074655000
C	-1.724878000	0.670877000	0.123632000
C	-2.114161000	1.463974000	1.261465000
C	-2.314722000	-2.339876000	2.777590000
C	-2.359034000	-1.316527000	3.774932000
C	-1.097779000	-0.637651000	3.778995000
C	-0.249500000	-1.296085000	2.827499000
C	-1.025506000	-2.296012000	2.147814000
O	1.007584000	-1.002828000	2.472365000
O	3.667115000	-0.019027000	1.946416000
O	3.850563000	0.223872000	-0.710685000
O	1.624328000	1.146664000	-2.133741000
O	-0.560285000	0.793608000	-0.523437000
C	4.549789000	-0.933073000	1.230804000
C	5.054769000	-0.088286000	0.047564000
C	3.958503000	1.328425000	-1.619272000
C	2.973045000	1.053095000	-2.758832000
C	0.656237000	0.192444000	-2.606094000
C	-0.685540000	0.755965000	-2.126460000
C	1.746164000	-0.070283000	3.346179000
C	3.215250000	-0.494886000	3.246838000
H	-3.998638000	1.438455000	2.492567000

H	-4.701742000	-0.674203000	0.946260000
H	-2.705886000	-1.140968000	-0.803998000
H	-1.552801000	2.301406000	1.664238000
H	-3.115483000	-3.030656000	2.530320000
H	-3.203105000	-1.078532000	4.415645000
H	-0.838862000	0.195986000	4.423815000
H	-0.659767000	-2.947886000	1.360568000
H	3.946969000	-1.775669000	0.855027000
H	5.706136000	-0.708736000	-0.588623000
H	4.973926000	1.356634000	-2.044360000
H	3.112232000	0.015077000	-3.086651000
H	0.840385000	-0.786382000	-2.129752000
H	-1.505292000	0.053096000	-2.307283000
H	1.398107000	-0.251302000	4.371980000
H	3.252748000	-1.592877000	3.254572000
Na	1.880245000	1.094942000	0.313707000
N	1.528194000	1.286371000	2.884336000
H	2.394188000	1.827982000	2.927136000
H	0.826274000	1.778350000	3.437247000
N	3.941156000	-0.020865000	4.375491000
H	4.023143000	0.995036000	4.426304000
H	4.870969000	-0.439167000	4.408228000
N	5.585439000	-1.443372000	2.078812000
H	6.442941000	-0.889871000	2.052807000
H	5.798653000	-2.424900000	1.915685000
N	5.775435000	1.083390000	0.457177000
H	6.773891000	1.061532000	0.271784000
H	5.568459000	1.383278000	1.408800000
N	3.605577000	2.549603000	-0.881017000
H	3.348360000	3.309648000	-1.515863000
H	4.441696000	2.848613000	-0.370111000
N	3.185588000	1.908191000	-3.864479000
H	3.048792000	2.900987000	-3.680431000
H	2.643268000	1.622862000	-4.678096000
N	0.683082000	0.019235000	-4.029181000
H	0.054349000	0.648587000	-4.528750000
H	0.560773000	-0.942260000	-4.336442000
N	-0.947736000	2.003267000	-2.646609000
H	-1.885237000	2.382823000	-2.562724000
H	-0.196305000	2.684314000	-2.567615000

$2_{\text{Fe}}(\text{d}) \cdots \text{Na}^+ / \text{BP86-D3(BJ)/Def2-TZVP}$

Fe	-1.303350000	0.015358000	1.434811000
C	-2.974948000	2.362420000	2.036126000
C	-3.775650000	1.591274000	1.228987000
C	-2.945350000	0.927867000	0.230830000
C	-1.660888000	1.562017000	0.331433000
C	-1.594583000	2.239587000	1.585394000
C	-2.312579000	-1.566689000	2.213457000
C	-1.951621000	-0.633978000	3.238126000
C	-0.518154000	-0.495219000	3.223306000
C	-0.020078000	-1.351456000	2.183871000
C	-1.127040000	-2.026977000	1.553647000
O	1.287794000	-1.408071000	1.755782000
O	3.714230000	-0.390266000	2.300639000
O	3.882855000	0.611740000	-0.202086000
O	1.693276000	0.744532000	-1.849489000
O	-0.472789000	1.006154000	-0.203632000
C	4.936121000	0.189803000	1.869932000
C	4.581951000	1.291736000	0.845190000
C	4.013095000	1.165103000	-1.528580000
C	3.017569000	0.352953000	-2.367490000
C	0.683473000	-0.280231000	-1.914439000
C	-0.631945000	0.445048000	-1.609233000
C	2.227150000	-2.201801000	2.639261000
C	3.614254000	-1.859465000	2.091171000
H	-3.298615000	2.981992000	2.868239000
H	-4.855011000	1.485179000	1.298130000
H	-3.326945000	0.349575000	-0.606012000
H	-0.753648000	2.828623000	1.942064000
H	-3.330151000	-1.840442000	1.949650000
H	-2.645233000	-0.089259000	3.871042000
H	0.077732000	0.154386000	3.856483000
H	-1.058694000	-2.737296000	0.735714000
H	5.539261000	-0.546460000	1.307643000
H	5.514081000	1.723023000	0.434799000
H	5.030817000	0.970960000	-1.901318000
H	3.155887000	-0.718301000	-2.161615000
H	0.876908000	-1.036964000	-1.131725000
H	-1.446724000	-0.286532000	-1.537695000
H	1.996960000	-3.258006000	2.449477000

H	3.648182000	-2.022182000	1.002789000
Na	1.789355000	0.736623000	0.926823000
N	2.160029000	-1.934497000	4.018802000
H	2.381253000	-0.969298000	4.257433000
H	1.314259000	-2.258490000	4.480478000
N	4.583974000	-2.663621000	2.725853000
H	4.566832000	-2.566837000	3.741327000
H	5.527793000	-2.557731000	2.361697000
N	5.696934000	0.591380000	3.034775000
H	5.156417000	1.199314000	3.652305000
H	6.575136000	1.052695000	2.790641000
N	3.685658000	2.299988000	1.417376000
H	3.692118000	3.112329000	0.792775000
H	4.027750000	2.603668000	2.333206000
N	3.783117000	2.593547000	-1.536494000
H	4.393274000	3.087027000	-2.184466000
H	2.806599000	2.824408000	-1.725374000
N	3.226290000	0.590511000	-3.752746000
H	3.094900000	1.572019000	-4.001546000
H	2.595708000	0.012084000	-4.308142000
N	0.645256000	-0.944317000	-3.192912000
H	-0.016207000	-0.490960000	-3.827571000
H	0.433845000	-1.936911000	-3.114822000
N	-0.910503000	1.425624000	-2.573665000
H	-1.823592000	1.864104000	-2.473620000
H	-0.166920000	2.116905000	-2.661830000

2_{Fe}⁺(e)---Na⁺ / BP86-D3(BJ)/Def2-TZVP

Fe	-1.668926000	-0.999574000	1.807208000
C	-3.139080000	0.533853000	1.891185000
C	-3.658100000	-0.556696000	1.133805000
C	-2.785474000	-0.805801000	0.034027000
C	-1.727849000	0.162600000	0.110224000
C	-1.934037000	0.989853000	1.271344000
C	-1.520737000	-3.001006000	2.262893000
C	-1.786352000	-2.237516000	3.444380000
C	-0.692640000	-1.329076000	3.650181000
C	0.277810000	-1.613829000	2.635914000
C	-0.262767000	-2.571340000	1.725572000
O	1.511253000	-1.092346000	2.444527000

O	4.038218000	0.405422000	2.204823000
O	3.624321000	0.587437000	-0.668497000
O	1.421066000	1.115482000	-2.245605000
O	-0.672264000	0.267723000	-0.775087000
C	4.740939000	-0.350016000	1.269405000
C	4.860610000	0.497926000	0.004119000
C	3.475563000	-0.064153000	-1.886089000
C	2.645795000	0.799530000	-2.842373000
C	0.239770000	0.724238000	-2.885925000
C	-0.904330000	1.024036000	-1.921797000
C	1.990885000	-0.131343000	3.343494000
C	3.523662000	-0.201641000	3.345078000
H	-3.573435000	0.933169000	2.804276000
H	-4.541028000	-1.139711000	1.384212000
H	-2.890821000	-1.585901000	-0.715474000
H	-1.305285000	1.816056000	1.586161000
H	-2.160264000	-3.769063000	1.836755000
H	-2.662124000	-2.317533000	4.082717000
H	-0.612598000	-0.614578000	4.464476000
H	0.240295000	-2.938460000	0.835354000
H	4.251407000	-1.302497000	1.019328000
H	5.681498000	0.140574000	-0.631955000
H	2.570985000	0.352830000	-3.838727000
H	0.232077000	-0.341060000	-3.161071000
H	-1.884403000	0.871673000	-2.393808000
H	1.593969000	-0.224905000	4.362031000
H	3.849268000	-1.238702000	3.495080000
Na	2.085736000	2.863868000	-0.177202000
N	1.602445000	1.292234000	2.840984000
O	1.730715000	2.191292000	3.646637000
O	1.248927000	1.392522000	1.660974000
N	4.035745000	0.566343000	4.625986000
O	4.783412000	1.501177000	4.458196000
O	3.591675000	0.096185000	5.666095000
N	6.165421000	-0.778310000	1.774622000
O	6.906621000	-1.202987000	0.901979000
O	6.349356000	-0.723973000	2.977104000
N	5.253077000	1.943702000	0.448833000
O	6.368167000	2.044514000	0.908114000
O	4.410614000	2.832048000	0.324551000

N	3.457688000	2.120951000	-3.027884000
O	4.446982000	2.012920000	-3.724924000
O	3.067852000	3.112664000	-2.420119000
N	0.007113000	1.476683000	-4.243810000
O	0.898701000	2.224076000	-4.613827000
O	-1.034811000	1.184498000	-4.802121000
N	-0.857755000	2.574357000	-1.599111000
O	-1.397733000	3.296501000	-2.406938000
O	-0.264006000	2.917240000	-0.571239000
H	4.423180000	-0.380740000	-2.348736000
N	2.651620000	-1.394951000	-1.657200000
O	2.632939000	-1.848833000	-0.523226000
O	2.094534000	-1.850669000	-2.646036000

2_{Fe}(e)⁻Na⁺ / BP86-D3(BJ)/Def2-TZVP

Fe	-1.667654000	-0.841989000	1.654016000
C	-3.240162000	-1.399730000	0.450303000
C	-2.262335000	-2.442126000	0.509916000
C	-1.014067000	-1.922084000	0.038054000
C	-1.244252000	-0.556183000	-0.309663000
C	-2.614238000	-0.213582000	-0.053311000
C	-2.238887000	-1.134661000	3.614743000
C	-2.330043000	0.253378000	3.274747000
C	-1.041812000	0.706880000	2.848173000
C	-0.172054000	-0.430808000	2.910478000
C	-0.894961000	-1.572226000	3.395051000
O	1.198800000	-0.431985000	2.577137000
O	3.944179000	-0.564921000	2.221404000
O	3.562635000	0.476795000	-0.418655000
O	1.575414000	1.851342000	-2.086588000
O	-0.249400000	0.239343000	-0.904482000
C	4.078271000	-1.300846000	1.051743000
C	4.616958000	-0.372385000	-0.026494000
C	3.806953000	1.328761000	-1.514852000
C	2.689822000	1.155896000	-2.544321000
C	0.339118000	1.642478000	-2.707852000
C	-0.718737000	1.302073000	-1.653751000
C	2.049510000	-0.377934000	3.684154000
C	3.309884000	-1.160941000	3.321152000
H	-4.275479000	-1.477384000	0.767729000

H	-2.430066000	-3.450836000	0.874731000
H	-0.075748000	-2.458995000	-0.059449000
H	-3.098096000	0.748821000	-0.194118000
H	-3.061643000	-1.761835000	3.944805000
H	-3.230944000	0.858321000	3.311852000
H	-0.783884000	1.716476000	2.543101000
H	-0.500638000	-2.573887000	3.539165000
H	3.132111000	-1.753495000	0.712627000
H	5.033459000	-0.951160000	-0.863050000
H	4.790438000	1.187991000	-1.974687000
H	2.496436000	0.083251000	-2.706789000
H	0.358665000	0.855622000	-3.472520000
H	-1.694812000	1.127728000	-2.124308000
H	1.596036000	-0.755906000	4.609182000
H	3.036580000	-2.209142000	3.152950000
Na	1.636423000	1.438152000	0.914341000
N	2.425034000	1.113096000	4.003700000
O	2.180472000	1.958286000	3.138544000
O	2.934945000	1.307679000	5.087345000
N	4.280610000	-1.203452000	4.544006000
O	5.334553000	-0.611208000	4.455793000
O	3.832009000	-1.853277000	5.480838000
N	5.029385000	-2.550035000	1.190060000
O	5.302753000	-3.096054000	0.130731000
O	5.321440000	-2.896630000	2.319430000
N	5.836034000	0.421306000	0.558620000
O	5.821231000	1.636448000	0.440749000
O	6.705207000	-0.285184000	1.037732000
N	3.759388000	2.814842000	-1.037176000
O	4.260946000	3.609527000	-1.805201000
O	3.185093000	3.049875000	0.021478000
N	3.191579000	1.641495000	-3.957453000
O	4.297682000	1.230520000	-4.274516000
O	2.407190000	2.299052000	-4.617316000
N	-0.124974000	2.932673000	-3.463247000
O	0.393264000	3.984294000	-3.144885000
O	-1.012559000	2.722634000	-4.278835000
N	-0.966155000	2.553837000	-0.718049000
O	-1.849070000	3.314714000	-1.056708000
O	-0.250972000	2.656564000	0.282651000

$2_{\text{Fe}}^+(\text{a})$ / BP86–D3(BJ)/Def2–TZVP

Fe	-1.523090000	-0.224671000	1.708364000
C	-2.662173000	1.448164000	1.321035000
C	-3.489710000	0.293005000	1.489872000
C	-3.133330000	-0.664082000	0.479324000
C	-2.150607000	-0.043662000	-0.365918000
C	-1.795083000	1.222444000	0.202643000
C	-1.317001000	-0.666313000	3.696531000
C	-0.355944000	0.313767000	3.286526000
C	0.475279000	-0.268348000	2.270727000
C	0.091017000	-1.648507000	2.147297000
C	-1.081929000	-1.861209000	2.943675000
O	0.563311000	-2.594315000	1.346342000
O	3.235193000	-1.763283000	2.446138000
O	3.274431000	0.410281000	0.571273000
O	1.005771000	0.816919000	-1.213827000
O	-1.625234000	-0.665359000	-1.427639000
C	4.320736000	-0.841237000	2.315007000
C	3.890594000	0.539207000	1.851534000
C	2.946800000	1.648319000	-0.051855000
C	2.330280000	1.341664000	-1.396012000
C	0.532717000	0.134116000	-2.373523000
C	-0.977396000	0.155522000	-2.439835000
C	1.756134000	-2.310406000	0.556837000
C	3.014401000	-2.639899000	1.344180000
H	-2.670090000	2.338357000	1.942762000
H	-4.251923000	0.152940000	2.250481000
H	-3.577677000	-1.640521000	0.314418000
H	-1.008587000	1.876661000	-0.157676000
H	-2.098882000	-0.528992000	4.437313000
H	-0.270956000	1.327289000	3.667031000
H	1.290220000	0.203733000	1.734739000
H	-1.633543000	-2.794184000	3.003547000
H	5.078327000	-1.244346000	1.621500000
H	4.782911000	-0.748061000	3.309752000
H	3.186157000	0.992604000	2.575546000
H	4.782026000	1.192494000	1.792985000
H	3.855334000	2.261279000	-0.199724000
H	2.242783000	2.231464000	0.574181000
H	2.287772000	2.259149000	-2.010722000

H	2.965524000	0.603531000	-1.916887000
H	0.906923000	-0.906253000	-2.387175000
H	0.892119000	0.632103000	-3.293700000
H	-1.360952000	1.183425000	-2.372572000
H	-1.296218000	-0.283113000	-3.395133000
H	1.745324000	-1.266410000	0.219692000
H	1.673579000	-2.985705000	-0.304851000
H	2.928014000	-3.661897000	1.747416000
H	3.866058000	-2.619268000	0.642314000

2_{Fe}(a) / BP86–D3(BJ)/Def2–TZVP

Fe	-1.605848000	-0.671262000	1.578725000
C	-2.725584000	-0.749169000	-0.131331000
C	-1.473852000	-1.431870000	-0.313790000
C	-0.408842000	-0.504344000	-0.074430000
C	-1.014233000	0.752853000	0.271390000
C	-2.445760000	0.610138000	0.227201000
C	-2.575350000	-1.724487000	3.038787000
C	-2.542062000	-0.325061000	3.351803000
C	-1.169439000	0.089368000	3.426217000
C	-0.360127000	-1.069944000	3.173156000
C	-1.223014000	-2.184318000	2.909888000
O	0.996889000	-1.187725000	3.198746000
O	3.614530000	-0.676391000	1.571630000
O	2.850396000	-1.316630000	-1.173091000
O	1.886458000	1.525613000	-1.158888000
O	-0.327066000	1.896765000	0.620171000
C	3.156278000	-1.965206000	1.162098000
C	3.557828000	-2.181453000	-0.283381000
C	3.571743000	-0.133166000	-1.529284000
C	2.612207000	0.840114000	-2.174942000
C	0.685788000	2.107124000	-1.637285000
C	-0.039090000	2.774205000	-0.483521000
C	1.726740000	0.041391000	3.014826000
C	3.204151000	-0.283633000	2.876569000
H	-3.712044000	-1.195225000	-0.223182000
H	-1.355563000	-2.480498000	-0.572531000
H	0.659275000	-0.690090000	-0.151576000
H	-3.167473000	1.386392000	0.464186000
H	-3.468545000	-2.326971000	2.901282000

H	-3.405776000	0.320096000	3.486695000
H	-0.815437000	1.100219000	3.600543000
H	-0.891143000	-3.188685000	2.665600000
H	2.061531000	-2.043122000	1.255433000
H	3.607473000	-2.754870000	1.798685000
H	4.649018000	-2.056454000	-0.403498000
H	3.300038000	-3.214975000	-0.566729000
H	4.377219000	-0.388110000	-2.246373000
H	4.022550000	0.331509000	-0.637663000
H	3.172529000	1.563845000	-2.799867000
H	1.919169000	0.282864000	-2.833772000
H	0.046146000	1.331732000	-2.101374000
H	0.888505000	2.880126000	-2.408276000
H	0.583303000	3.568449000	-0.049977000
H	-0.973815000	3.222162000	-0.869887000
H	1.576185000	0.690263000	3.896883000
H	1.354330000	0.567586000	2.119259000
H	3.782166000	0.625598000	3.096594000
H	3.477018000	-1.056361000	3.622209000

2_{Fe}⁺(b) / BP86–D3(BJ)/Def2–TZVP

Fe	-1.785461000	-0.686540000	1.978531000
C	-2.445315000	1.281814000	1.466128000
C	-3.342037000	0.260274000	0.986080000
C	-2.590213000	-0.621340000	0.129152000
C	-1.225385000	-0.117573000	0.084415000
C	-1.161319000	1.100331000	0.855037000
C	-2.494525000	-2.410026000	2.842728000
C	-2.891301000	-1.276299000	3.650086000
C	-1.709590000	-0.568250000	4.043443000
C	-0.564725000	-1.327815000	3.571209000
C	-1.050475000	-2.517332000	2.941576000
O	0.719144000	-1.112999000	3.995995000
O	3.187058000	-0.570314000	1.361321000
O	4.169964000	0.385748000	-1.287172000
O	1.477000000	1.725130000	-1.439474000
O	-0.222133000	-0.600057000	-0.711764000
C	3.866937000	-1.369890000	0.392773000
C	4.835379000	-0.506110000	-0.392595000
C	3.836388000	1.653911000	-0.715758000

C	2.782352000	2.316970000	-1.577433000
C	1.265210000	0.565569000	-2.256774000
C	-0.129167000	0.042769000	-2.022812000
C	1.598414000	-0.380570000	3.110017000
C	2.150566000	-1.283915000	2.016389000
H	3.135538000	-1.828405000	-0.299970000
H	4.420999000	-2.187234000	0.897189000
H	5.497549000	0.047426000	0.296536000
H	5.463468000	-1.161093000	-1.014975000
H	4.733982000	2.303240000	-0.678864000
H	3.451378000	1.528778000	0.308943000
H	2.668349000	3.365878000	-1.266585000
H	3.084689000	2.302189000	-2.638654000
H	2.012893000	-0.208355000	-2.029091000
H	1.366646000	0.842837000	-3.322935000
H	-0.869272000	0.855730000	-2.083271000
H	-0.366336000	-0.714477000	-2.785791000
H	2.419916000	-0.024990000	3.745262000
H	1.068811000	0.480469000	2.675729000
H	2.551661000	-2.209041000	2.480578000
H	1.357338000	-1.561997000	1.295879000
N	-0.049406000	1.885466000	0.991000000
H	-0.184192000	2.829637000	1.337393000
H	0.639111000	1.808243000	0.224557000
N	-2.813355000	2.276501000	2.387264000
H	-2.333199000	3.165393000	2.249281000
H	-3.823583000	2.436075000	2.365781000
N	-4.701738000	0.226818000	1.297641000
H	-4.848056000	0.055751000	2.310847000
H	-5.191729000	-0.499430000	0.775413000
N	-3.128192000	-1.749393000	-0.532023000
H	-2.383780000	-2.326470000	-0.927425000
H	-3.777371000	-1.500019000	-1.281853000
N	-1.702611000	0.577445000	4.840322000
H	-2.130386000	1.385080000	4.363366000
H	-0.762237000	0.812963000	5.157563000
N	-0.344216000	-3.542913000	2.412521000
H	0.622757000	-3.674354000	2.685909000
H	-0.880480000	-4.357312000	2.123730000
N	-4.196619000	-0.879191000	3.963959000

H	-4.220127000	-0.339527000	4.832245000
H	-4.850470000	-1.659724000	4.014944000
N	-3.278508000	-3.396528000	2.204450000
H	-3.623615000	-3.093480000	1.284740000
H	-4.032651000	-3.778087000	2.773743000

2_{Fe}(b) / BP86–D3(BJ)/Def2–TZVP

Fe	-1.530533000	-0.148192000	1.693123000
C	-3.093442000	1.189309000	1.491726000
C	-3.330009000	-0.053129000	0.799018000
C	-2.255687000	-0.259414000	-0.167805000
C	-1.368520000	0.876145000	-0.040586000
C	-1.869381000	1.744980000	0.999265000
C	-1.413512000	-2.012479000	2.458502000
C	-1.888971000	-1.072949000	3.453216000
C	-0.902608000	-0.033819000	3.595608000
C	0.208087000	-0.370507000	2.715198000
C	-0.090695000	-1.605449000	2.045469000
O	1.371048000	0.367248000	2.591636000
O	4.227917000	-1.055005000	2.941051000
O	2.934807000	-1.110151000	-0.441422000
O	1.050602000	0.127615000	-3.320163000
O	-0.215950000	1.161110000	-0.737826000
C	4.055077000	-1.588397000	1.625827000
C	3.714922000	-0.506139000	0.596321000
C	2.519015000	-0.149000000	-1.416086000
C	1.491740000	-0.808757000	-2.326882000
C	-0.282300000	0.604245000	-3.143935000
C	-0.422232000	1.677680000	-2.074712000
C	2.250457000	0.235067000	3.730814000
C	3.062363000	-1.055978000	3.765695000
H	3.250456000	-2.342377000	1.620142000
H	5.000096000	-2.089340000	1.369681000
H	3.124571000	0.289179000	1.080276000
H	4.627913000	-0.053434000	0.166031000
H	3.388394000	0.197531000	-2.006428000
H	2.062754000	0.718646000	-0.911586000
H	1.951067000	-1.662259000	-2.852555000
H	0.640117000	-1.176596000	-1.732708000
H	-0.961903000	-0.233713000	-2.912692000

H	-0.569322000	1.045509000	-4.112735000
H	0.345810000	2.452409000	-2.224533000
H	-1.420136000	2.145378000	-2.140162000
H	1.653163000	0.305887000	4.657391000
H	2.930903000	1.097401000	3.684045000
H	3.429896000	-1.189036000	4.797497000
H	2.409984000	-1.913404000	3.519500000
N	-1.106806000	1.144982000	4.373139000
H	-0.911262000	1.974096000	3.797422000
H	-0.506904000	1.178926000	5.200902000
N	-3.166834000	-1.094532000	4.072445000
H	-3.222277000	-0.295175000	4.710726000
H	-3.308671000	-1.951732000	4.611064000
N	-2.083129000	-3.124463000	1.871856000
H	-3.058176000	-2.887389000	1.654833000
H	-2.050052000	-3.967612000	2.448623000
N	0.727751000	-2.357676000	1.211408000
H	1.355073000	-1.814020000	0.607631000
H	0.177107000	-3.019082000	0.661936000
N	-1.254297000	2.912382000	1.525478000
H	-1.766919000	3.760943000	1.271450000
H	-0.300923000	2.988007000	1.163844000
N	-3.917257000	1.781707000	2.459499000
H	-3.357285000	2.220641000	3.194757000
H	-4.535678000	1.092201000	2.889807000
N	-4.339597000	-1.013356000	1.104069000
H	-5.236720000	-0.800107000	0.662391000
H	-4.468159000	-1.065720000	2.124021000
N	-2.082089000	-1.372142000	-1.044080000
H	-2.875386000	-1.451253000	-1.686053000
H	-2.063632000	-2.236740000	-0.491573000

2_{Fe}^{+(c)} / BP86–D3(BJ)/Def2–TZVP

Fe	-1.630503000	-0.403160000	2.010811000
C	-2.145518000	1.523061000	2.365798000
C	-3.126396000	0.897712000	1.543402000
C	-2.473693000	0.479018000	0.332954000
C	-1.131052000	1.011204000	0.311811000
C	-0.910889000	1.546053000	1.630228000
C	-1.911662000	-2.417878000	1.851530000

C	-2.465875000	-1.927999000	3.073953000
C	-1.396298000	-1.379631000	3.859247000
C	-0.141350000	-1.617911000	3.164740000
C	-0.506291000	-2.176402000	1.896731000
O	1.119390000	-1.511627000	3.499501000
O	2.509031000	0.280200000	1.976445000
O	3.507535000	-0.795652000	-0.665657000
O	1.504875000	-0.101776000	-2.735748000
O	-0.203666000	0.999747000	-0.616304000
C	3.555225000	0.773905000	1.142962000
C	3.199627000	0.549295000	-0.312466000
C	3.625909000	-1.037302000	-2.058349000
C	2.265162000	-1.299589000	-2.727129000
C	0.084067000	-0.252105000	-2.710306000
C	-0.511658000	0.970852000	-2.054469000
C	1.724046000	-0.334285000	4.140134000
C	2.933861000	0.018012000	3.313107000
H	4.508922000	0.271774000	1.381076000
H	3.676649000	1.860550000	1.305859000
H	2.120804000	0.734564000	-0.470492000
H	3.758850000	1.247732000	-0.958463000
H	4.233877000	-1.945586000	-2.167927000
H	4.122450000	-0.188851000	-2.558334000
H	2.491661000	-1.609152000	-3.765738000
H	1.726518000	-2.106634000	-2.210423000
H	-0.213327000	-1.175096000	-2.193184000
H	-0.299313000	-0.294391000	-3.746860000
H	-0.036770000	1.881911000	-2.441096000
H	-1.590109000	1.037311000	-2.226894000
H	2.006036000	-0.617379000	5.160052000
H	0.991820000	0.476394000	4.172072000
H	3.405247000	0.910082000	3.765637000
H	3.672760000	-0.803751000	3.313261000
N	0.273641000	2.284620000	2.066232000
O	0.413822000	2.412102000	3.283466000
O	1.002017000	2.741359000	1.192499000
N	-2.410559000	2.277317000	3.622806000
O	-2.485869000	3.485105000	3.452395000
O	-2.529778000	1.642511000	4.656160000
N	-4.573614000	0.812231000	1.797626000

O	-5.001583000	1.536247000	2.686777000
O	-5.194845000	0.039314000	1.076766000
N	-3.141409000	-0.086102000	-0.864351000
O	-3.895821000	0.682020000	-1.446482000
O	-2.813462000	-1.217223000	-1.204661000
N	-1.546715000	-0.962192000	5.261045000
O	-0.550868000	-0.487271000	5.801726000
O	-2.640911000	-1.163660000	5.768874000
N	0.486963000	-2.548375000	0.881575000
O	0.509778000	-1.855470000	-0.135743000
O	1.210198000	-3.490216000	1.154111000
N	-3.842408000	-2.222187000	3.571067000
O	-4.666114000	-1.327880000	3.557051000
O	-3.964252000	-3.375005000	3.957638000
N	-2.632037000	-3.184366000	0.827401000
O	-3.854500000	-3.113816000	0.862360000
O	-1.929806000	-3.824703000	0.050170000

2_{Fe(c)} / BP86–D3(BJ)/Def2–TZVP

Fe	0.565598000	-0.121006000	0.461613000
C	-3.282725000	-0.086248000	0.589229000
C	-2.816757000	-1.195846000	-0.174164000
C	-1.581543000	-0.845107000	-0.720364000
C	-1.211134000	0.501945000	-0.240569000
C	-2.359529000	0.949654000	0.526455000
C	-2.002518000	-0.676080000	4.742786000
C	-1.322069000	0.519305000	4.583684000
C	-0.477667000	0.388740000	3.424734000
C	-0.664858000	-0.918848000	2.896649000
C	-1.627442000	-1.572652000	3.692294000
O	0.104116000	-1.445299000	1.888596000
O	2.827484000	-1.657728000	2.547645000
O	2.836854000	0.126050000	0.156473000
O	1.863762000	1.611878000	-2.956078000
O	-0.302658000	1.335406000	-0.871539000
C	3.976227000	-1.032903000	1.979412000
C	3.663988000	0.303423000	1.340059000
C	2.936877000	1.257411000	-0.763972000
C	2.728960000	0.761229000	-2.203337000
C	0.554392000	1.117080000	-3.205696000

C	-0.496623000	1.706803000	-2.287457000
C	0.773045000	-2.752589000	2.114972000
C	2.209848000	-2.622207000	1.701918000
H	4.469141000	-1.702116000	1.253547000
H	4.682952000	-0.847909000	2.803675000
H	3.153800000	0.978083000	2.042980000
H	4.611216000	0.770883000	1.024283000
H	3.934906000	1.700311000	-0.637052000
H	2.190759000	2.021452000	-0.500206000
H	3.691101000	0.745150000	-2.735925000
H	2.343417000	-0.269376000	-2.172596000
H	0.541266000	0.015361000	-3.182308000
H	0.280187000	1.428846000	-4.228324000
H	-0.444949000	2.802727000	-2.284422000
H	-1.503476000	1.383631000	-2.587524000
H	0.229043000	-3.501808000	1.531518000
H	0.677370000	-2.963054000	3.186749000
H	2.685298000	-3.616616000	1.811619000
H	2.279247000	-2.332904000	0.640164000
N	0.477017000	1.294198000	2.996904000
O	0.867577000	1.243807000	1.732974000
O	0.959969000	2.154527000	3.718654000
N	-1.623995000	1.733068000	5.309215000
O	-1.522326000	2.797709000	4.694863000
O	-1.987103000	1.601477000	6.482858000
N	-3.010666000	-0.949507000	5.778246000
O	-4.128545000	-0.481298000	5.609885000
O	-2.616791000	-1.621636000	6.725446000
N	-2.270522000	-2.815230000	3.404362000
O	-1.982226000	-3.364751000	2.320532000
O	-3.085827000	-3.250166000	4.218476000
N	-2.532134000	2.262013000	1.102717000
O	-3.353242000	2.361631000	2.017994000
O	-1.848047000	3.177811000	0.631540000
N	-4.524794000	-0.090116000	1.380371000
O	-5.486667000	0.469315000	0.873171000
O	-4.468235000	-0.659323000	2.462621000
N	-3.443497000	-2.503164000	-0.220992000
O	-4.643174000	-2.537707000	0.066835000
O	-2.742579000	-3.454247000	-0.565322000

N	-0.633612000	-1.618673000	-1.421587000
O	-0.867030000	-2.369781000	-2.350437000
O	0.589214000	-1.375879000	-0.995199000

2_{Fe}⁺(d) / BP86–D3(BJ)/Def2–TZVP

Fe	-2.132794000	0.184045000	1.882803000
C	-3.091157000	1.989454000	1.693539000
C	-3.750840000	0.988613000	0.911774000
C	-2.823672000	0.497591000	-0.067658000
C	-1.609052000	1.251241000	0.068708000
C	-1.747168000	2.113891000	1.210758000
C	-2.826746000	-1.393657000	2.991609000
C	-2.334268000	-0.363024000	3.852315000
C	-0.940906000	-0.164808000	3.569790000
C	-0.553128000	-1.138755000	2.586635000
C	-1.741327000	-1.834005000	2.163786000
O	0.613524000	-1.338113000	1.993570000
O	4.129713000	-0.504428000	2.175958000
O	3.969516000	0.554288000	-0.420334000
O	1.573549000	1.047523000	-2.445213000
O	-0.450921000	1.114305000	-0.562964000
C	5.216922000	-0.578020000	1.236174000
C	5.153826000	0.708906000	0.381030000
C	3.556406000	1.744014000	-1.123052000
C	3.017496000	1.306527000	-2.507805000
C	1.195719000	-0.134600000	-1.744832000
C	-0.324928000	0.001961000	-1.549036000
C	1.789364000	-0.543947000	2.474320000
C	2.975531000	-1.284956000	1.825982000
H	-3.523824000	2.548660000	2.517490000
H	-4.776779000	0.652733000	1.029185000
H	-3.033496000	-0.257363000	-0.815754000
H	-0.960904000	2.753652000	1.597315000
H	-3.842148000	-1.776691000	2.960865000
H	-2.910866000	0.188639000	4.588814000
H	-0.297780000	0.577978000	4.024756000
H	-1.768283000	-2.615770000	1.411294000
H	5.085853000	-1.449204000	0.572265000
H	6.038311000	0.752439000	-0.282387000
H	4.449298000	2.360389000	-1.296930000

H	3.507903000	0.367967000	-2.800301000
H	1.672577000	-0.175458000	-0.753136000
H	-0.707301000	-0.904265000	-1.055194000
H	1.829974000	-0.681562000	3.566858000
H	2.842079000	-1.270391000	0.732798000
N	1.617505000	0.825506000	2.158186000
H	2.020038000	1.144467000	1.261958000
H	1.938773000	1.436462000	2.904334000
N	3.019856000	-2.650703000	2.268923000
H	3.329743000	-2.701703000	3.242393000
H	3.668152000	-3.206692000	1.710778000
N	6.438359000	-0.760409000	1.978239000
H	6.752290000	0.114719000	2.403845000
H	7.186775000	-1.121596000	1.387223000
N	5.122778000	1.925423000	1.162275000
H	6.049170000	2.316685000	1.319225000
H	4.641238000	1.774088000	2.050989000
N	2.558925000	2.462464000	-0.356329000
H	1.695673000	2.607008000	-0.882228000
H	2.923242000	3.327858000	0.035303000
N	3.280888000	2.317974000	-3.476638000
H	2.824951000	3.201155000	-3.238863000
H	2.976083000	2.034197000	-4.407564000
N	1.588306000	-1.313933000	-2.478672000
H	0.972896000	-1.504802000	-3.271137000
H	1.664750000	-2.141146000	-1.888801000
N	-1.077944000	0.293252000	-2.714073000
H	-1.581584000	-0.490797000	-3.115641000
H	-0.547478000	0.816361000	-3.409999000

2_{Fe}(d) / BP86–D3(BJ)/Def2–TZVP

Fe	-1.699152000	-0.705757000	1.415404000
C	-3.186838000	0.418635000	2.240378000
C	-3.533039000	0.013516000	0.910974000
C	-2.534295000	0.527320000	0.013056000
C	-1.592226000	1.283416000	0.798741000
C	-1.975038000	1.185909000	2.173260000
C	-1.628913000	-2.696037000	0.953153000
C	-1.708476000	-2.503242000	2.371346000
C	-0.569287000	-1.735640000	2.785598000

C	0.225697000	-1.465225000	1.615965000
C	-0.441197000	-2.042527000	0.484772000
O	1.407038000	-0.809739000	1.514679000
O	4.093543000	-0.033567000	2.863063000
O	3.845147000	0.161868000	0.004112000
O	1.761606000	1.276367000	-1.613010000
O	-0.540104000	2.058501000	0.382237000
C	4.582064000	-1.041532000	1.932917000
C	5.052970000	-0.287859000	0.680729000
C	3.990851000	0.335031000	-1.387971000
C	2.604296000	0.158669000	-2.034463000
C	0.370673000	1.005926000	-1.686489000
C	-0.384438000	2.210599000	-1.072393000
C	1.657210000	0.241123000	2.543382000
C	2.796742000	-0.238878000	3.462137000
H	-3.730039000	0.170577000	3.147505000
H	-4.388291000	-0.593016000	0.627097000
H	-2.513467000	0.369105000	-1.060452000
H	-1.439543000	1.636066000	3.003903000
H	-2.347897000	-3.228878000	0.337582000
H	-2.501181000	-2.861653000	3.022265000
H	-0.351050000	-1.418818000	3.800980000
H	-0.081160000	-2.004717000	-0.539557000
H	3.750073000	-1.706024000	1.660847000
H	5.563065000	-0.997820000	0.007909000
H	4.618623000	-0.473594000	-1.804686000
H	2.150109000	-0.764818000	-1.641025000
H	0.130821000	0.112668000	-1.084942000
H	-1.407790000	2.217582000	-1.479561000
H	0.737850000	0.326439000	3.135867000
H	2.665498000	-1.316058000	3.669519000
N	1.967909000	1.494756000	1.966458000
H	1.163599000	1.852930000	1.446303000
H	2.757021000	1.387872000	1.321224000
N	2.702134000	0.505150000	4.688893000
H	2.727682000	1.502826000	4.455995000
H	3.508813000	0.302191000	5.281906000
N	5.681504000	-1.810097000	2.450917000
H	5.422196000	-2.278852000	3.319529000
H	6.469035000	-1.183446000	2.637219000

N	5.973089000	0.750101000	1.055777000
H	5.515466000	1.356116000	1.742080000
H	6.201295000	1.311622000	0.232489000
N	4.665755000	1.597674000	-1.694599000
H	5.063326000	1.584591000	-2.635051000
H	4.004408000	2.375295000	-1.631635000
N	2.770471000	0.034562000	-3.458699000
H	3.199460000	0.888116000	-3.827012000
H	1.839851000	-0.040342000	-3.879459000
N	-0.047964000	0.741232000	-3.067329000
H	-0.144347000	1.626597000	-3.573802000
H	-0.953270000	0.267406000	-3.078631000
N	0.261430000	3.429662000	-1.398826000
H	1.246660000	3.401614000	-1.136179000
H	-0.199838000	4.232624000	-0.973583000

$2_{\text{Fe}^+}(\text{e}) / \text{BP86-D3(BJ)/Def2-TZVP}$

Fe	-1.523262000	-1.015948000	1.165132000
C	-3.108180000	0.360793000	1.499415000
C	-3.516712000	-0.736093000	0.677724000
C	-2.699451000	-0.740096000	-0.500551000
C	-1.811515000	0.386715000	-0.396095000
C	-2.061166000	1.060982000	0.838202000
C	-0.903804000	-2.969026000	1.005915000
C	-1.482427000	-2.721087000	2.294480000
C	-0.688465000	-1.725043000	2.957049000
C	0.433904000	-1.455093000	2.100009000
C	0.260691000	-2.151078000	0.870200000
O	1.515192000	-0.670863000	2.275491000
O	3.805910000	0.764537000	2.446679000
O	3.441860000	0.120135000	-0.351327000
O	1.699907000	1.422169000	-2.742669000
O	-0.898689000	0.655949000	-1.377017000
C	4.649157000	-0.009911000	1.651869000
C	4.638323000	0.539180000	0.233213000
C	3.371438000	0.083319000	-1.739791000
C	1.881940000	0.208250000	-2.092357000
C	0.402131000	1.941848000	-2.857521000
C	-0.426322000	1.963776000	-1.565306000
C	1.744961000	0.027239000	3.478415000

C	3.265162000	0.192937000	3.587661000
H	-3.509256000	0.615937000	2.476072000
H	-4.301377000	-1.450578000	0.909033000
H	-2.751031000	-1.424417000	-1.342078000
H	-1.520074000	1.902709000	1.255996000
H	-1.277813000	-3.655780000	0.252147000
H	-2.372272000	-3.190166000	2.704152000
H	-0.879983000	-1.294638000	3.934050000
H	0.923036000	-2.101739000	0.008545000
H	4.350360000	-1.069067000	1.606374000
H	5.543628000	0.221560000	-0.302413000
H	1.323484000	0.120423000	-1.152985000
H	-0.180761000	1.429982000	-3.637241000
H	-1.231353000	2.709291000	-1.627494000
H	1.332781000	-0.475036000	4.361923000
H	3.708880000	-0.782045000	3.836166000
N	0.986462000	1.388735000	3.394239000
O	1.616131000	2.422040000	3.476770000
O	-0.231222000	1.263829000	3.241178000
N	3.576811000	1.066632000	4.851756000
O	4.390782000	1.950879000	4.759672000
O	2.935221000	0.705688000	5.841036000
N	6.107003000	-0.082716000	2.230846000
O	6.997935000	-0.319512000	1.429917000
O	6.190187000	0.004333000	3.445696000
N	4.708869000	2.103754000	0.270908000
O	3.903972000	2.711038000	-0.420762000
O	5.604041000	2.558504000	0.963766000
N	1.310959000	-0.991248000	-2.913253000
O	1.319203000	-2.059018000	-2.298133000
O	0.831503000	-0.772502000	-4.009049000
N	0.552994000	3.404951000	-3.378727000
O	1.669109000	3.821957000	-3.595973000
O	-0.524856000	3.967002000	-3.546263000
N	0.487551000	2.452271000	-0.391062000
O	0.746237000	3.639621000	-0.404606000
O	0.850635000	1.611277000	0.430541000
H	3.930123000	0.884772000	-2.243238000
N	4.024523000	-1.238180000	-2.281469000
O	4.562118000	-1.972041000	-1.466373000

O 3.971421000 -1.365901000 -3.495666000

$2_{Fe}(e)$ / BP86-D3(BJ)/Def2-TZVP

Fe -1.554779000 -0.932970000 1.523787000
C -3.007790000 -1.475676000 0.199002000
C -2.000736000 -2.490701000 0.281372000
C -0.744433000 -1.910973000 -0.091348000
C -0.995046000 -0.546444000 -0.424586000
C -2.385558000 -0.253134000 -0.225942000
C -2.386095000 -1.138375000 3.389055000
C -2.214810000 0.250023000 3.071203000
C -0.828580000 0.493716000 2.814193000
C -0.159198000 -0.763017000 2.966779000
C -1.106377000 -1.778592000 3.328998000
O 1.204581000 -0.985430000 2.759316000
O 4.113519000 -0.692273000 2.509929000
O 3.632976000 1.171711000 -0.453063000
O 1.839961000 2.095034000 -2.354793000
O 0.001349000 0.238239000 -0.989469000
C 3.520845000 -0.394463000 1.294887000
C 4.449407000 0.495015000 0.448279000
C 3.957202000 1.158695000 -1.799540000
C 2.657068000 0.998373000 -2.580250000
C 0.472108000 1.914225000 -2.579574000
C -0.303537000 1.548177000 -1.306404000
C 2.032573000 -0.861405000 3.867372000
C 3.386611000 -1.448276000 3.450842000
H -4.059002000 -1.592977000 0.444733000
H -2.154711000 -3.517043000 0.600305000
H 0.222577000 -2.401449000 -0.142926000
H -2.891666000 0.697354000 -0.362370000
H -3.330312000 -1.629198000 3.606516000
H -3.007987000 0.989796000 3.014354000
H -0.354102000 1.432440000 2.553669000
H -0.888071000 -2.829303000 3.494627000
H 2.531150000 0.076989000 1.359096000
H 5.273910000 -0.057054000 -0.022833000
H 4.660245000 0.362771000 -2.086292000
H 2.204916000 0.045486000 -2.265942000
H 0.259015000 1.158840000 -3.347130000

H	-1.372664000	1.746872000	-1.447050000
H	1.652026000	-1.347166000	4.776681000
H	3.226545000	-2.477583000	3.103355000
N	2.255637000	0.635484000	4.286895000
O	2.022127000	1.501061000	3.458137000
O	2.676901000	0.783506000	5.428293000
N	4.295398000	-1.596883000	4.693129000
O	5.336966000	-0.973315000	4.733012000
O	3.849683000	-2.383457000	5.525724000
N	3.285396000	-1.702357000	0.450450000
O	2.663354000	-1.563499000	-0.601025000
O	3.726117000	-2.753938000	0.893006000
N	5.157361000	1.519017000	1.401066000
O	6.316713000	1.243227000	1.680458000
O	4.490596000	2.466323000	1.773626000
N	4.705482000	2.483672000	-2.176890000
O	4.587876000	2.862281000	-3.334298000
O	5.384690000	2.977386000	-1.290800000
N	2.949015000	0.780506000	-4.102988000
O	3.844849000	-0.018621000	-4.354056000
O	2.208814000	1.341235000	-4.895269000
N	-0.098073000	3.227825000	-3.183768000
O	0.657320000	4.159874000	-3.360422000
O	-1.297004000	3.160038000	-3.449894000
N	0.146487000	2.514896000	-0.162635000
O	-0.275608000	3.661515000	-0.273692000
O	0.869141000	2.069373000	0.712945000