Supplementary Material

to the article entitled

"The Reactivity of Human and Equin Estrogen-quinones towards Purine Nucleosides"

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1. Command lines for Gaussian16 calculations

1.1. Intermediates (minima on potential energy hypersurface)

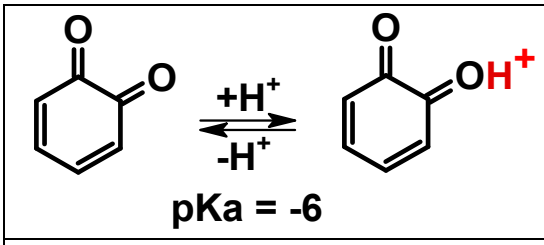
```
# B3LYP/6-311++G** opt freq=noraman integral=(acc2e=12)
scf=xqc scrf=cpcm empiricaldispersion=gd3bj
```

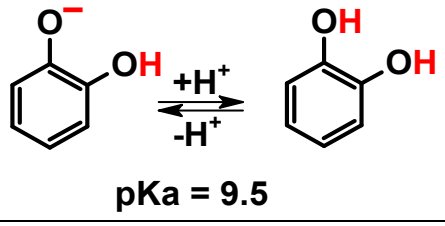
1.2. Transition states (first order saddle points on potential energy hypersurface)

```
# B3LYP/6-311++G** opt=(TS, calcfc, noeigentest) freq=noraman
integral=(acc2e=12) scf=xqc scrf=cpcm
empiricaldispersion=gd3bj
```

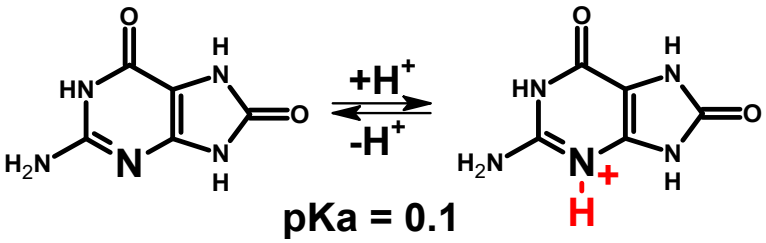
(Note: the temperature for thermochemical analysis is set to 25°C by default. For calculations at 37°C, “temperature=310.15” was added to the command line.)

2. List of reference acids used for pK_a calculations

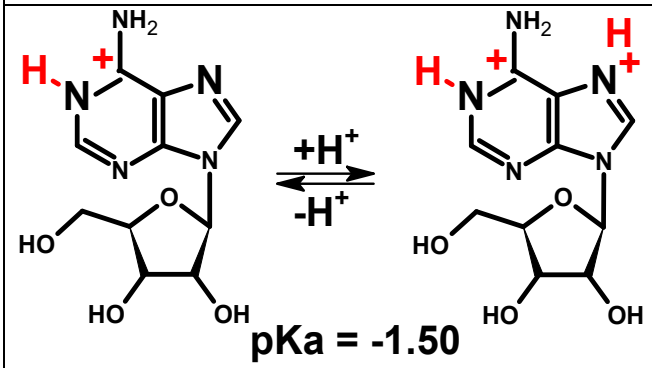




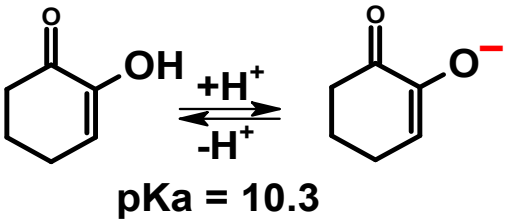
ortho-Quinone (left), **Cathecol** (right): T. Palomäki *et al.*, "Electrochemical reactions of catechol, methylcatechol and dopamine at tetrahedral amorphous carbon (ta-C) thin film electrodes," *Diam. Relat. Mater.*, vol. 59, pp. 30–39, 2015, doi: 10.1016/j.diamond.2015.09.003.



8-Oxo-guanine: S. Raoul and J. Cadet, "Photosensitized reaction of 8-oxo-7,8-dihydro-2'-deoxyguanosine: Identification of 1-(2-deoxy-β-D-erythro-pentofuranosyl)cyanuric acid as the major singlet oxygen oxidation product," *J. Am. Chem. Soc.*, vol. 118, no. 8, pp. 1892–1898, 1996, doi: 10.1021/ja952347l.



Adenosine-1,7-H: G. Kampf, L. E. Kapinos, R. Griesser, B. Lippert, and H. Sigel, "Comparison of the acid-base properties of purine derivatives in aqueous solution. Determination of intrinsic proton affinities of various basic sites," *J. Chem. Soc. Perkin Trans. 2*, no. 7, pp. 1320–1327, 2002, doi: 10.1039/B202023H.



Cyclohexan-1,2-dione: Yannai S.: Dictionary of Food Compounds: Additives, Flavors, and Ingredients (Chapman & Hall/CRC Press, 2004), 225.

3. Details of pK_a calculations

Table S1. Molecular Gibbs free energy (G) of reference acids ("Ref_aH^+") and their conjugate base forms ("Ref_a").

Acid (Ref_aH^+)	G (Ref_aH^+) [E_h]	G (Ref_a) [E_h]
AcOH	-229.145592	-228.691086
ortho-Quinone	-381.918633	-381.530258
Cathecol	-382.301626	-382.761271
8-Oxo-guanine	-618.381938	-617.96352
Adenosine-1,7-H	-964.538769	-964.130947
Cyclohexan-1,2-dione	-383.933194	-383.456004

Table S2. Molecular Gibbs free energy (G) of initial intermediates ("Int") of elementary steps, and their conjugate acid forms ("$IntH^+$"). The calculation of pK_a of $IntH^+$ was based on the following steps (see the "Computational Methods" section of the article for mathematical details):

$$\Delta G_a = G(Int) + G(Ref_aH^+) - G(IntH^+) - G(Ref_a)$$

$$pK_a(IntH^+) = pK_a(Ref_aH^+) + 0.732\,\Delta G_a$$

(ΔG_a is to be substituted to the above expression in kcal/mol unit. 1 E_h = 627.5 kcal/mol)

Base-acid pair Int / $IntH^+$	G(Int) [E_h]	G($IntH^+$) [E_h]	Reference acid	ΔG_a [kcal/mol]	pK_a ($IntH^+$)
E'-Q(H) / E'-Q(H)H^+	-616.174712	-616.569411	**ortho-Quinone**	-3.97	-3.1
Eq'-Q(H) / Eq'-Q(H)H^+	-614.970456	-615.363195	**ortho-Quinone**	-2.74	-4.0
Eqn'-Q(H) / Eqn'-Q(H)H^+	-613.815836	-614.218768	**ortho-Quinone**	-9.13	0.7
E'-Q(H)$^-$-G^+R / E'-Q(H)H-G^+R	-1390.080196	-1390.540276	**Cyclohexan-1,2-dione**	10.74	2.4
Eq'-Q(H)$^-$-G^+R / Eq'-Q(H)H-G^+R	-1388.873884	-1389.335882	**Cyclohexan-1,2-dione**	9.53	3.3
Eqn'-Q(H)$^-$-G^+R / Eqn'-Q(H)H-G^+R	-1387.717429	-1388.177421	**Cyclohexan-1,2-dione**	10.79	2.4
E'-Q(H)$^-$-A^+R / E'-Q(H)H-A^+R	-1314.792896	-1315.254642	**Cyclohexan-1,2-dione**	9.69	3.2
Eq'-Q(H)$^-$-A^+R / Eq'-Q(H)H-A^+R	-1313.587933	-1314.046569	**Cyclohexan-1,2-dione**	11.64	1.8
Eqn'-Q(H)$^-$-A^+R / Eqn'-Q(H)H-A^+R	-1312.433456	-1312.874904	**Cyclohexan-1,2-dione**	11.63	1.8
E'-QH$^-$-G^+R' / E'-QH_2-G^+R'	-1390.104270	-1390.558782	**Cathecol**	3.22	6.9
Eq'-QH$^-$-G^+R' / Eq'-QH_2-G^+R'	-1388.905671	-1389.356374	**Cathecol**	5.61	5.1
Eqn'-QH$^-$-G^+R' / Eqn'-QH_2-G^+R'	-1387.729369	-1388.176351	**Cathecol**	7.95	3.4
E'-QH$^-$-A^+R' / E'-QH_2-A^+R'	-1314.831239	-1315.283045	**Cathecol**	4.92	5.6
Eq'-QH$^-$-A^+R' / Eq'-QH_2-A^+R'	-1313.631532	-1314.080391	**Cathecol**	6.77	4.3
Eqn'-QH$^-$-A^+R' / Eqn'-QH_2-A^+R'	-1312.456155	-1312.900464	**Cathecol**	9.62	2.2
E'-QH_2-G^+R' / E'-QH_2-GH^{2+}R'	-1390.558782	-1390.965880	**8-Oxo-guanine**	7.10	-5.1
E'-QH_2-G^+R' / E'-QH_2-GH^{2+}R'	-1389.356374	-1389.763011	**8-Oxo-guanine**	7.39	-5.3
E'-QH_2-G^+R' / E'-QH_2-GH^{2+}R'	-1388.176351	-1388.583033	**8-Oxo-guanine**	7.36	-5.3
E'-QH_2-A^+R' / E'-QH_2-AH^{2+}R'	-1315.283045	-1315.688204	**adenosine**	1.67	-2.7
Eq'-QH_2-A^+R' / Eq'-QH_2-AH^{2+}R'	-1314.080391	-1314.487692	**adenosine**	0.33	-1.7
Eqn'-QH_2-A^+R' / Eqn'-QH_2-AH^{2+}R'	-1312.900464	-1313.308422	**adenosine**	-0.09	-1.4

Table S3. Protonated fraction (x_{prot}) of initial intermediates of elementary steps, and the value of the corresponding Gibbs free energy correction of -RTln(x_{prot}). The calculation of x_{prot} was based on the following formula (see the "Computational Methods" section of the article for mathematical details):

$$x_{prot} = 10^{pK_a(IntH^+)-7.2} \text{ or}$$

$$x_{prot} = 10^{pK_a\left(IntH_2^{2+}\right)+pK_a(IntH^+)-14.4} \text{ (in the case of double protonation)}$$

Protonated intermediate $IntH^+$	x_{prot}	-RTln(x_{prot}) [kcal/mol]
E'-Q(H)H$^+$	5.07E-11	14.1
Eq'-Q(H)H$^+$	6.37E-12	15.3
Eqn'-Q(H)H$^+$	3.07E-07	8.9
E'-Q(H)H-G$^+$R	1.74E-05	6.5
Eq'-Q(H)H-G$^+$R	1.33E-04	5.3
Eqn'-Q(H)H-G$^+$R	1.58E-05	6.6
E'-Q(H)H-A$^+$R	1.02E-04	5.4
Eq'-Q(H)H-A$^+$R	3.78E-06	7.4
Eqn'-Q(H)H-A$^+$R	3.88E-06	7.4
E'-QH$_2$-G$^+$R'	2.76E-01	0.8
Eq'-QH$_2$-G$^+$R'	8.64E-03	2.8
Eqn'-QH$_2$-G$^+$R'	1.71E-04	5.1
E'-QH$_2$-A$^+$R'	2.69E-02	2.1
Eq'-QH$_2$-A$^+$R'	1.24E-03	4.0
Eqn'-QH$_2$-A$^+$R'	1.02E-05	6.8
E'-QH$_2$-GH^{2+}R'	1.39E-13	17.5
Eq'-QH$_2$-GH^{2+}R'	2.66E-15	19.9
Eqn'-QH$_2$-GH^{2+}R'	5.52E-17	22.2
E'-QH$_2$-AH^{2+}R'	3.21E-12	15.7
Eq'-QH$_2$-AH^{2+}R'	1.43E-12	16.2
Eqn'-QH$_2$-AH^{2+}R'	2.34E-14	18.6

4. Details of the calculation of Gibbs free energy changes, barriers and effective barriers

Table S4. Molecular Gibbs free energy (G) of common reactant molecules, used for the calculation of Gibbs free energy profiles.

Molecule	G [E_h]
GR'	-773.936029
AR'	-698.663869
CH_3COO^-	-228.691086
CH_3COOH	-229.145592
R^{+}'	-231.657713

Table S5. Molecular Gibbs free energy (G) of initial intermediate species, transition states and products presented in Figures 7a and 7c.

Estrogen (Ex')	G(Q(H)) [E_h]	G(Q(H)H^+) [E_h]	G(TS) (Q(H)-GR') [E_h]
E'	-616.174712	-616.569411	-1390.074569
Eq'	-614.970456	-615.363195	-1388.872944
Eqn'	-613.815836	-614.218768	-1387.715806

Estrogen (Ex')	G(TS) (Q(H)H^+-GR') [E_h]	G (Q(H)-GR') [E_h]	G (Q(H)H^+-GR') [E_h]
E'	-1390.504614	-1390.080196	-1390.540276
Eq'	-1389.299842	-1388.873884	-1389.335882
Eqn'	-1388.149179	-1387.717429	-1388.177421

Table S6. Calculation of relative Gibbs free energies (G_{rel}) visualized in Figure 7c. The following formulas were used (see the "Computational Methods" section of the article for mathematical details):

G_{rel}(Ex'-Q(H)H^+) = -RTln(x_{prot})

G_{rel}(Ex'-Q(H)-GR'(TS)) = G(Ex'-Q(H)-GR'(TS)) – G(Ex'-Q(H)) – G(GR')

G_{rel}(Ex'-Q(H)H^+-GR'(TS)) = G(Ex'-Q(H)H^+-GR'(TS)) – G(Ex'-Q(H)H^+) – G(GR') + G_{rel}(Ex'-Q(H)H^+)

G_{rel}(Ex'-Q(H)-GR') = G(Ex'-Q(H)-GR') – G(Ex'-Q(H)) – G(GR')

G_{rel}(Ex'-Q(H)H^+-GR') = G(Ex'-Q(H)H^+-GR') – G(Ex'-Q(H)H^+) – G(GR') + G_{rel}(Ex'-Q(H)H^+)

Values of activation Gibbs free energies and effective activation Gibbs free energies relate to G_{rel} values as:

$\Delta G^{\ddagger}$(Ex'-Q(H) + GR') = G_{rel}(Ex'-Q(H)-GR'(TS))

$\Delta G^{\ddagger}$(Ex'-Q(H)H^+ + GR') = G_{rel}(Ex'-Q(H)H^+-GR'(TS)) - G_{rel}(Ex'-Q(H)H^+)

$\Delta G^{\ddagger}_{eff}$(Ex'-Q(H)$H^+$ + GR') = G_{rel}(Ex'-Q(H)H^+-GR'(TS))

	Gibbs free energy (G_{rel}) relative to the initial state (Ex'-Q(H) + GR'), in kcal/mol					
Estrogen (Ex')	**Q(H)**	**Q(H)H^+**	**Q(H)-GR' (TS)**	**Q(H)H^+-GR' (TS)**	**Q(H)-GR'**	**Q(H)H^+-GR'**
E'	0.0	14.1	22.7	14.6	19.2	-7.8
Eq'	0.0	15.3	21.0	15.3	20.5	-7.7
Eqn'	0.0	8.9	22.6	12.4	21.6	-5.3

Table S7. Molecular Gibbs free energy (G) of initial intermediate species, transition states and products presented in Figures 7b and 7d.

Estrogen (Ex')	G(Q(H)) [E_h]	G(Q(H)H^+) [E_h]	G(TS) (Q(H)-AR') [E_h]
E'	-616.174712	-616.569411	-1314.789891
Eq'	-614.970456	-615.363195	-1313.585704
Eqn'	-613.815836	-614.218768	-1312.430374

Estrogen (Ex')	G(TS) (Q(H)H^+-AR') [E_h]	G (Q(H)-AR') [E_h]	G (Q(H)H^+-AR') [E_h]
E'	-1315.227425	-1314.792896	-1315.254642
Eq'	-1314.022123	-1313.587933	-1314.046569
Eqn'	-1312.874904	-1312.433456	-1312.874904

Table S8. Calculation of relative Gibbs free energies (G_{rel}) visualized in Figure 7d. The following formulas were used (see the "Computational Methods" section of the article for mathematical details):

G_{rel}(Ex'-Q(H)H^+) = -RTln(x_{prot})

G_{rel}(Ex'-Q(H)-AR'(TS)) = G(Ex'-Q(H)-GR'(TS)) – G(Ex'-Q(H)) – G(AR')

G_{rel}(Ex'-Q(H)H^+-AR'(TS)) = G(Ex'-Q(H)H^+-AR'(TS)) – G(Ex'-Q(H)H^+) – G(AR') + G_{rel}(Ex'-Q(H)H^+)

G_{rel}(Ex'-Q(H)-AR') = G(Ex'-Q(H)-AR') – G(Ex'-Q(H)) – G(AR')

G_{rel}(Ex'-Q(H)H^+-AR') = G(Ex'-Q(H)H^+-AR') – G(Ex'-Q(H)H^+) – G(AR') + G_{rel}(Ex'-Q(H)H^+)

Values of activation Gibbs free energies and effective activation Gibbs free energies relate to G_{rel} values as:

$\Delta G^{\ddagger}$(Ex'-Q(H) + AR') = G_{rel}(Ex'-Q(H)-AR'(TS))

$\Delta G^{\ddagger}$(Ex'-Q(H)H^+ + AR') = G_{rel}(Ex'-Q(H)H^+-AR'(TS)) - G_{rel}(Ex'-Q(H)H^+)

$\Delta G^{\ddagger}_{eff}$(Ex'-Q(H)$H^+$ + AR') = G_{rel}(Ex'-Q(H)H^+-AR'(TS))

	Gibbs free energy (G_{rel}) relative to the initial state (Ex'-Q(H) + AR'), in kcal/mol					
Estrogen (Ex')	Q(H)	Q(H)H^+	Q(H)-AR' (TS)	Q(H)H^+-AR' (TS)	Q(H)-AR'	Q(H)H^+-AR'
E'	0.0	14.1	30.6	17.6	28.7	0.7
Eq'	0.0	15.3	30.5	18.4	29.1	3.1
Eqn'	0.0	8.9	31.0	13.8	29.0	3.0

Table S9. Molecular Gibbs free energy (G) of initial intermediate species, transition states and products presented in Figures 9a and 9c.

Estrogen (Ex')	G(Ex'-Q(H)$^-$-G$^+$R') [E_h]	G(Ex'-Q(H)H-G$^+$R') [E_h]	G(Ex'-Q(H)$^-$-G$^+$R' (TS)) [E_h]
E'	-1390.080196	-1390.540276	-1618.734217
Eq'	-1388.873884	-1389.335882	-1617.531095
Eqn'	-1387.717429	-1388.177421	-1616.371569

Estrogen (Ex')	G(Ex'-Q(H)H$^+$-GR' (TS)) [E_h]	G(Ex'-Q^{2-}-G$^+$R') [E_h]	G(Ex'-QH$^-$-G$^+$R') [E_h]
E'	-1619.213562	-1389.612021	-1390.104270
Eq'	-1618.010320	-1388.413478	-1388.905671
Eqn'	-1616.848886	-1387.240974	-1387.729369

Table S10. Calculation of relative Gibbs free energies (G_{rel}) visualized in Figure 9c. The following formulas were used (see the "Computational Methods" section of the article for mathematical details):

G_{rel}(Ex'-Q(H)H-G$^+$R'$^+$) = -RTln(x_{prot})

G_{rel}(Ex'-Q(H)$^-$-G$^+$R' (TS)) = G(Ex'-Q(H)$^-$-G$^+$R' (TS)) – G(Ex'-Q(H)$^-$-G$^+$R') - G(acetate)

G_{rel}(Ex'-Q(H)H$^+$-GR' (TS)) = G(Ex'-Q(H)H$^+$-GR' (TS)) – G(Ex'-Q(H)H-G$^+$R') – G(acetate) + G_{rel}(Ex'-Q(H)H-G$^+$R')

G_{rel}(Ex'-Q^{2-}-G$^+$R') = G(Ex'-Q^{2-}-G$^+$R') + G(acetic acid) – G(Ex'-Q(H)$^-$-G$^+$R') – G(acetate)

G_{rel}(Ex'-QH$^-$-G$^+$R') = G(Ex'-QH$^-$-G$^+$R') + G(acetic acid) – G(Ex'-Q(H)H-G$^+$R') – G(acetate) + G_{rel}(Ex'-Q(H)H-G$^+$R')

Values of activation Gibbs free energies and effective activation Gibbs free energies relate to G_{rel} values as:

$\Delta G^{\ddagger}$(Ex'-Q(H)$^-$-G$^+$R') = G_{rel}(Ex'-Q(H)$^-$-G$^+$R' (TS))

$\Delta G^{\ddagger}$(Ex'-Q(H)H-G$^+$R') = G_{rel}(Ex'-Q(H)H$^+$-GR' (TS)) - G_{rel}(Ex'-Q(H)H-G$^+$R')

$\Delta G^{\ddagger}_{eff}$(Ex'-Q(H)H-G$^+$R') = G_{rel}(Ex'-Q(H)H$^+$-GR' (TS))

	Gibbs free energy (G_{rel}) relative to the initial state, in kcal/mol					
Estrogen (Ex')	Ex'-Q(H)$^-$-G$^+$R'	Ex'-Q(H)H-G$^+$R'	Ex'-Q(H)$^-$-G$^+$R' (TS)	Ex'-Q(H)H$^+$-GR' (TS)	Ex'-Q^{2-}-G$^+$R'	Ex'-QH$^-$-G$^+$R'
E'	0.0	6.5	23.3	17.7	8.6	-5.1
Eq'	0.0	5.3	21.3	15.8	3.7	-9.9
Eqn'	0.0	6.6	23.2	18.9	13.8	2.5

Table S11. Molecular Gibbs free energy (G) of initial intermediate species, transition states and products presented in Figures 9b and 9d.

Estrogen (Ex')	G(Ex'-Q(H)$^-$-A$^+$R') [E_h]	G(Ex'-Q(H)H-A$^+$R') [E_h]	G(Ex'-Q(H)$^-$-A$^+$R' (TS)) [E_h]
E'	-1314.792896	-1315.254642	-1543.454288
Eq'	-1313.587933	-1314.046569	-1542.252383
Eqn'	-1312.433456	-1312.874904	-1541.093178

Estrogen (Ex')	G(Ex'-Q(H)H$^+$-AR' (TS)) [E_h]	G(Ex'-Q^{2-}-A$^+$R') [E_h]	G(Ex'-QH$^-$-A$^+$R') [E_h]
E'	-1543.931493	-1314.341581	-1314.831239
Eq'	-1542.728943	-1313.142571	-1313.631532
Eqn'	-1541.570192	-1311.969271	-1312.456155

Table S12. Calculation of relative Gibbs free energies (G_{rel}) visualized in Figure 9d. The following formulas were used (see the "Computational Methods" section of the article for mathematical details):

G_{rel}(Ex'-Q(H)$^-$-A$^+$R') = -RTln(x_{prot})

G_{rel}(Ex'-Q(H)$^-$-A$^+$R' (TS)) = G(Ex'-Q(H)$^-$-A$^+$R' (TS)) – G(Ex'-Q(H)$^-$-A$^+$R') – G(acetate)

G_{rel}(Ex'-Q(H)H$^+$-AR' (TS)) = G(Ex'-Q(H)H$^+$-AR' (TS)) – G(Ex'-Q(H)H-A$^+$R') – G(acetate) + G_{rel}(Ex'-Q(H)H-A$^+$R')

G_{rel}(Ex'-Q^{2-}-A$^+$R') = G(Ex'-Q^{2-}-A$^+$R') + G(acetic acid) – G(Ex'-Q(H)$^-$-A$^+$R') – G(acetate)

G_{rel}(Ex'-QH$^-$-A$^+$R') = G(Ex'-QH$^-$-A$^+$R') + G(acetic acid) – G(Ex'-Q(H)H-A$^+$R') – G(acetate) + G_{rel}(Ex'-Q(H)H-A$^+$R')

Values of activation Gibbs free energies and effective activation Gibbs free energies relate to G_{rel} values as:

$\Delta G^{\ddagger}$(Ex'-Q(H)$^-$-A$^+$R') = G_{rel}(Ex'-Q(H)$^-$-A$^+$R' (TS))

$\Delta G^{\ddagger}$(Ex'-Q(H)H-A$^+$R') = G_{rel}(Ex'-Q(H)H$^+$-AR' (TS))- G_{rel}(Ex'-Q(H)H-A$^+$R')

$\Delta G^{\ddagger}_{eff}$(Ex'-Q(H)H-A$^+$R') = G_{rel}(Ex'-Q(H)H$^+$-AR' (TS))

	Gibbs free energy (G_{rel}) relative to the initial state, in kcal/mol					
Estrogen (Ex')	Q(H)	Q(H)H$^+$	Q(H)-AR' (TS)	Q(H)H$^+$-AR' (TS)	Q(H)-AR'	Q(H)H$^+$-AR'
E'	0.0	5.5	18.6	14.4	-2.0	-14.0
Eq'	0.0	7.4	16.7	12.9	-5.7	-17.3
Eqn'	0.0	7.4	19.7	15.6	6.1	-4.2

Table S13. Molecular Gibbs free energy (G) of initial intermediate species, transition states and products presented in Figures 10a, 10c and 10e.

Estrogen (Ex')	G(Ex'-QH$^-$-G$^+$R') [E_h]	G(Ex'-QH$_2$-G$^+$R') [E_h]	G(Ex'-QH$_2$-GH^{2+}R') [E_h]
E'	-1390.104270	-1390.558782	-1390.965880
Eq'	-1388.905671	-1389.356374	-1389.763011
Eqn'	-1387.729369	-1388.176351	-1388.583033

Estrogen (Ex')	G(Ex'-QH$_2$-GH^{2+}R' (TS)) [E_h]	G(Ex'-QH^{-}-G + R^{+}') [E_h]	G(Ex'-QH$_2$-G + R^{+}') [E_h]	G(Ex'-QH$_2$-GH$^+$ + R^{+}') [E_h]
E'	-1390.950254	-1158.415247	-1158.876356	-1159.304321
Eq'	-1389.745820	-1157.215581	-1157.672776	-1158.100915
Eqn'	-1388.566870	-1156.042410	-1156.495368	-1156.921690

Table S14. Calculation of relative Gibbs free energies (G_{rel}) visualized in Figures 10c and 10e. The following formulas were used (see the "Computational Methods" section of the article for mathematical details):

$G_{rel}(Ex'\text{-}QH_2\text{-}G^+R') = -RTln(x_{prot})$

$G_{rel}(Ex'\text{-}QH_2\text{-}GH^{2+}R') = -RTln(x_{prot})$

$G_{rel}(Ex'\text{-}QH_2\text{-}GH^{2+}R'\ (TS)) = G(Ex'\text{-}QH_2\text{-}GH^{2+}R'\ (TS)) - G(Ex'\text{-}QH_2\text{-}GH^{2+}R'\ ) + G_{rel}(Ex'\text{-}QH_2\text{-}GH^{2+}R')$

$G_{rel}(Ex'\text{-}QH^-\text{-}G + R^{+\cdot}) = G(Ex'\text{-}QH^-\text{-}G + R^{+\cdot}) - G(Ex'\text{-}QH^-\text{-}G^+R')$

$G_{rel}(Ex'\text{-}QH_2\text{-}G + R^{+\cdot}) = G(Ex'\text{-}QH_2\text{-}G + R^{+\cdot}) - G(Ex'\text{-}QH_2\text{-}G^+R') + G_{rel}(Ex'\text{-}QH_2\text{-}G^+R')$

$G_{rel}(Ex'\text{-}QH_2\text{-}GH^+ + R^{+\cdot}) = G(Ex'\text{-}QH_2\text{-}GH^+ + R^{+\cdot}) - G(Ex'\text{-}QH_2\text{-}GH^{2+}R') + G_{rel}(Ex'\text{-}QH_2\text{-}GH^{2+}R')$

Values of activation Gibbs free energies and effective activation Gibbs free energies relate to G_{rel} values as:

$\Delta G^{\ddagger}(Ex'\text{-}QH^{-\cdot}\text{-}G + R^{+\cdot}) = G_{rel}(Ex'\text{-}QH^{-\cdot}\text{-}G + R^{+\cdot}) - G_{rel}(Ex'\text{-}QH^-\text{-}G^+R')$

$\Delta G^{\ddagger}(Ex'\text{-}QH_2\text{-}G^+R') = G_{rel}(Ex'\text{-}QH_2\text{-}G + R^{+\cdot}) - G_{rel}(Ex'\text{-}QH_2\text{-}G^+R')$

$\Delta G^{\ddagger}_{eff}(Ex'\text{-}Q(H)H\text{-}G^+R') = G_{rel}(Ex'\text{-}QH_2\text{-}GH^{2+}R'\ (TS)) - G_{rel}(Ex'\text{-}QH_2\text{-}GH^+ + R')$

	Gibbs free energy (G_{rel}) relative to the initial state, in kcal/mol		
Estrogen (Ex')	**$Ex'\text{-}QH^-\text{-}G^+R'$**	**$Ex'\text{-}QH_2\text{-}G^+R'$**	**$Ex'\text{-}QH_2\text{-}GH^{2+}R'$**
E'	0	0.8	17.5
Eq'	0	2.8	19.9
Eqn'	0	5.2	22.2

	Gibbs free energy (G_{rel}) relative to the initial state, in kcal/mol			
Estrogen (Ex')	**$Ex'\text{-}QH_2\text{-}GH^{2+}R'$ (TS)**	**$Ex'\text{-}QH^-\text{-}G + R^{+\cdot}$**	**$Ex'\text{-}QH_2\text{-}G + R^{+\cdot}$**	**$Ex'\text{-}QH_2\text{-}GH^+ + R^{+\cdot}$**
E'	27.4	19.6	16.3	19.7
Eq'	30.7	20.3	19.1	22.3
Eqn'	32.4	18.4	19.7	24.2

Table S15. Molecular Gibbs free energy (G) of initial intermediate species, transition states and products presented in Figures 10b, 10d and 10f.

Estrogen (Ex')	**$G(Ex'\text{-}QH^-\text{-}A^+R')$ [E_h]**	**$G(Ex'\text{-}QH_2\text{-}A^+R')$ [E_h]**	**$G(Ex'\text{-}QH_2\text{-}AH^{2+}R')$ [E_h]**
E'	-1314.831239	-1315.283045	-1315.688204
Eq'	-1313.631532	-1314.080391	-1314.487692
Eqn'	-1312.456155	-1312.900464	-1313.308422

Estrogen (Ex')	**$G(Ex'\text{-}QH2\text{-}AH^{2+}R'$ (TS)) [E_h]**	**$G(Ex'\text{-}QH^-\text{-}A + R^{+\cdot})$ [E_h]**	**$G(Ex'\text{-}QH_2\text{-}A + R^{+\cdot})$ [E_h]**	**$G(Ex'\text{-}QH_2\text{-}AH^+ + R^{+\cdot})$ [E_h]**
E'	-1315.683848	-1083.139354	-1083.596083	-1084.035658
Eq'	-1314.483041	-1081.938002	-1082.392355	-1082.831131
Eqn'	-1313.302585	-1080.763323	-1081.214634	-1081.652998

Table S16. Calculation of relative Gibbs free energies (G_{rel}) visualized in Figure 10d and 10f. The following formulas were used (see the "Computational Methods" section of the article for mathematical details):

$G_{rel}(Ex'\text{-}QH_2\text{-}A^+R') = -RTln(x_{prot})$

$G_{rel}(Ex'\text{-}QH_2\text{-}AH^{2+}R') = -RTln(x_{prot})$

$G_{rel}(Ex'\text{-}QH_2\text{-}AH^{2+}R'\ (TS)) = G(Ex'\text{-}QH_2\text{-}AH^{2+}R'\ (TS)) - G(Ex'\text{-}QH_2\text{-}AH^{2+}R'\ ) + G_{rel}(Ex'\text{-}QH_2\text{-}AH^{2+}R')$

$G_{rel}(Ex'\text{-}QH^-\text{-}A + R') = G(Ex'\text{-}QH^-\text{-}A + R^{+}') - G(Ex'\text{-}QH^-\text{-}A^+R')$

$G_{rel}(Ex'\text{-}QH_2\text{-}A + R^{+}') = G(Ex'\text{-}QH_2\text{-}A + R^{+}') - G(Ex'\text{-}QH_2\text{-}A^+R') + G_{rel}(Ex'\text{-}QH_2\text{-}A^+R')$

$G_{rel}(Ex'\text{-}QH_2\text{-}AH^+ + R^{+}') = G(Ex'\text{-}QH_2\text{-}AH^+ + R^{+}') - G(Ex'\text{-}QH_2\text{-}AH^{2+}R') + G_{rel}(Ex'\text{-}QH_2\text{-}AH^{2+}R')$

Values of activation Gibbs free energies and effective activation Gibbs free energies relate to G_{rel} values as:

$\Delta G^{\ddagger}(Ex'\text{-}QH^-\text{-}A + R') = G_{rel}(Ex'\text{-}QH^-\text{-}A + R^{+}') - G_{rel}(Ex'\text{-}QH^-\text{-}A^+R')$

$\Delta G^{\ddagger}(Ex'\text{-}QH_2\text{-}A^+R') = G_{rel}(Ex'\text{-}QH_2\text{-}A + R^{+}') - G_{rel}(Ex'\text{-}QH_2\text{-}A^+R')$

$\Delta G^{\ddagger}_{eff}(Ex'\text{-}Q(H)H\text{-}A^+R') = G_{rel}(Ex'\text{-}QH_2\text{-}AH^{2+}R'\ (TS)) - G_{rel}(Ex'\text{-}QH_2\text{-}AH^+ + R^{+}')$

	Gibbs free energy (G_{rel}) relative to the initial state, in kcal/mol			
Estrogen (Ex')	**$Ex'\text{-}QH^-\text{-}A^+R'$**	**$Ex'\text{-}QH_2\text{-}A^+R'$**	**$Ex'\text{-}QH_2\text{-}AH^{2+}R'$**	**$Ex'\text{-}QH_2\text{-}AH^{2+}R'$ (TS)**
E'	0	2.2	15.7	18.5
Eq'	0	4.0	16.2	19.1
Eqn'	0	6.8	18.6	22.3

	Gibbs free energy (G_{rel}) relative to the initial state, in kcal/mol		
Estrogen (Ex')	**$Ex'\text{-}QH^-\text{-}A + R^{+}'$**	**$Ex'\text{-}QH_2\text{-}A + R^{+}'$**	**$Ex'\text{-}QH_2\text{-}AH^+ + R^{+}'$**
E'	21.4	20.5	12.4
Eq'	22.5	23.0	15.5
Eqn'	22.0	24.5	17.2

5. Investigation of the effect of temperature (25 °C vs 37 °C)

Table S17. Temperature dependence of selected activation Gibbs free energies and reaction Gibbs free energies. Calculations for 37°C were performed following the protocol presented in the previous sections, with the exception that "temperature=310.15" was added to the command line of input files.

Reaction	$\Delta G^{\ddagger}$ [kcal/mol]		ΔG [kcal/mol]	
	@ 25°C	@ 37 °C (deviation from 25 °C)	@ 25 °C	@ 37 °C (deviation from 25 °C)
E'-Q(H)H^+ + GR' → E'-Q(H)H^+-GR' (Michael addition)	0.5	1.0 (+ 0.5)	-21.9	-21.3 (+ 0.6)
E'-Q(H)H^+-GR' + AcO^-→ E'-QH^--G^+R' + AcOH (rearomatization)	11.2	11.6 (+ 0.4)	-11.6	-11.6 (0.0)
E'-QH_2-G^+R' → E'-QH_2-G + R'$^+$ (depurination)	-	-	15.5	15.0 (-0.5)
Average absolute deviation: 0.4 kcal/mol				
Eq'-Q(H)H^+ + GR' → Eq'-Q(H)H^+-GR' (Michael addition)	0.0	0.1 (+ 0.1)	-23.0	-22.5 (+ 0.5)
Eq'-Q(H)H^+-GR' + AcO^-→ Eq'-QH^--G^+R' + AcOH (rearomatization)	10.4	10.9 (+ 0.5)	-15.2	-15.3 (0.0)
Eq'-QH_2-G^+R' → Eq'-QH_2-G + R'$^+$ (depurination)	-	-	16.2	15.9 (- 0.4)
Average absolute deviation: 0.3 kcal/mol				
Eqn'-Q(H)H^+ + GR' → Eqn'-Q(H)H^+-GR' (Michael addition)	3.5	4.0 (+ 0.5)	-14.2	-13.7 (+ 0.5)
Eqn'-Q(H)H^+-GR' + AcO^-→ Eqn'-QH^--G^+R' + AcOH (rearomatization)	12.3	12.8 (+ 0.4)	-4.0	-4.1 (0.1)
Eqn'-QH_2-G^+R' → Eqn'-QH_2-G + R'$^+$ (depurination)	-	-	14.6	14.1 (- 0.5)
Average absolute deviation: 0.4 kcal/mol				

6. Optimized geometries

AcOH (Ref_a)	**AcOH (Ref_aH^+)**
C -1.350400 0.042276 -0.000004	C 1.391994 -0.122952 -0.000101
H -1.732933 -0.482859 0.879888	H 1.667010 -0.707035 -0.881059
H -1.732873 -0.483237 -0.879692	H 1.667845 -0.706726 0.880799
H -1.731269 1.064344 -0.000233	H 1.925779 0.824196 -0.000524
C 0.187607 0.000617 0.000026	C -0.087852 0.122867 0.000586
O 0.717409 -1.145395 -0.000006	O -0.790172 -1.031305 -0.000070
O 0.804320 1.100944 -0.000005	H -1.735532 -0.812503 -0.000391
	O -0.628572 1.206627 -0.000147
ortho-Quinone (Ref_a)	**ortho-Quinone-H^+ (Ref_aH^+)**
C 0.635363 -1.455428 0.000329	C 0.838197 1.411327 0.000027
C -0.665095 -0.783749 0.000007	C -0.511470 0.848696 -0.000214
C -0.664961 0.783782 0.000166	C -0.638714 -0.689814 -0.000180
C 0.635599 1.455350 -0.000327	C 0.493573 -1.507908 0.000002
C 1.770967 0.731137 -0.000217	C 1.710853 -0.878844 0.000071
C 1.770823 -0.731332 0.000194	C 1.887647 0.570248 0.000017
O -1.727572 -1.376395 -0.000525	O -1.550014 1.470900 0.000077
O -1.727319 1.376633 0.000434	O -1.830345 -1.155612 0.000091
H 0.638749 -2.538558 0.000518	H 0.935972 2.488288 0.000151
H 2.732513 -1.230737 0.000325	H -2.477921 -0.412772 0.000126
H 0.638939 2.538480 -0.000602	H 2.900283 0.950419 0.000064
H 2.732753 1.230352 -0.000427	H 0.395847 -2.584505 0.000032
	H 2.608168 -1.485966 -0.000056
cyclohexan-1,2-dione (Ref_a)	**cyclohexan-1,2-dione (Ref_aH^+)**
C 1.742546 0.969623 -0.000211	C -1.761874 -0.987811 -0.000160
C 1.942335 -0.565026 0.000551	C -1.978043 0.547438 0.000463
C 0.661747 -1.427793 -0.000224	C -0.718342 1.448502 -0.000355
C -0.704145 -0.755721 0.000069	C 0.632249 0.784194 -0.000047
C -0.845330 0.739191 0.000004	C 0.730319 -0.678933 0.000121
C 0.325095 1.461155 -0.000402	C -0.350146 -1.471857 -0.000176
H 2.264223 1.398280 0.866587	H -2.263491 -1.433213 0.866512
H 2.543938 -0.840347 -0.868114	H -2.582894 0.807996 -0.868538
H 0.650850 -2.094180 -0.869139	H -0.718646 2.112043 -0.870238
O -2.040392 1.239999 0.000429	O 2.003233 -1.175619 0.000146
O -1.692863 -1.490152 -0.000220	O 1.673495 1.440968 0.000069
H 0.650633 -2.095251 0.867849	H -0.718514 2.113271 0.868582
H 2.542442 -0.839700 0.870455	H -2.581467 0.807489 0.870609
H 2.264273 1.397600 -0.867312	H -2.263440 -1.432640 -0.867156
H 0.216189 2.546248 -0.000718	H 2.589265 -0.398985 -0.000156
	H -0.199607 -2.547949 -0.000420
Cathecol$^-$ (Ref_a)	**Cathecol (Ref_aH^+)**
C 0.624312 -1.406808 -0.000007	C -0.720983 -1.389273 -0.000037
C -0.545590 -0.674437 0.000001	C 0.500376 -0.726584 -0.000012
C 1.862360 -0.735152 -0.000002	C -1.911027 -0.659549 -0.000009
C -0.570327 0.760841 0.000007	C 0.532368 0.675456 0.000035
O -1.788100 -1.263130 0.000006	O 1.664633 -1.445000 0.000067
C 1.881750 0.657485 0.000003	C -1.877754 0.732990 -0.000004
C 0.690467 1.397855 0.000003	C -0.651894 1.402453 0.000057
O -1.736954 1.338689 -0.000011	O 1.788552 1.230532 -0.000081
H 0.579969 -2.491512 -0.000020	H -0.727142 -2.472725 -0.000073
H -2.377041 -0.475562 0.000024	H 2.407380 -0.825488 -0.000073
H 2.785893 -1.302488 0.000001	H 1.739842 2.193430 0.000064
H 2.832013 1.182712 0.000006	H -2.859127 -1.183244 -0.000040
H 0.721771 2.483681 0.000000	H -2.797815 1.304248 -0.000015
	H -0.615123 2.486553 0.000064
8-Oxo-guanine (Ref_a)	**8-Oxo-guanine-H^+ (Ref_aH^+)**
N 1.927451 0.673876 -0.001726	N 1.923299 0.715947 -0.002905
C 1.987780 -0.693226 -0.001258	C 2.052489 -0.623698 -0.000575
N 0.908033 -1.456199 0.002503	N 0.924820 -1.371994 -0.002710
C -0.245182 -0.766474 -0.001824	C -0.292597 -0.744567 -0.002224
C -0.394342 0.608576 -0.000902	C -0.427301 0.617243 0.000062
C 0.739130 1.449399 0.000315	C 0.703666 1.475398 -0.000622
N -1.510205 -1.306204 -0.000142	N -1.527115 -1.307439 -0.002079
C -2.481521 -0.297536 0.001288	C -2.513130 -0.292569 0.000700

N -1.765213 0.877979 0.002849 O 0.798686 2.681602 0.001806 N 3.213599 -1.270259 -0.050370 H 2.785429 1.212044 -0.023172 H 3.244644 -2.262735 0.126696 H 4.031056 -0.744296 0.217498 O -3.696148 -0.449412 0.001383 H -2.196891 1.788574 -0.002502 H -1.735397 -2.289886 -0.001552	N -1.793219 0.881965 0.001769 O 0.750509 2.691340 0.000175 N 3.242113 -1.203140 0.001721 H 2.765476 1.281562 -0.007390 H 3.339902 -2.207733 0.006069 H 4.090373 -0.657073 0.024366 H 0.986136 -2.382725 0.002632 O -3.717028 -0.458345 0.002222 H -2.221450 1.795176 0.004461 H -1.756326 -2.291385 -0.003937
Adenosine (Ref_a) N 4.352612 0.953664 -0.037585 C 3.414956 1.953345 0.012039 N 2.129989 1.753429 -0.014856 C 1.792787 0.449799 -0.100412 C 2.665590 -0.639017 -0.162235 C 4.044546 -0.376864 -0.127313 N 0.538263 -0.092118 -0.145535 C 0.707767 -1.462500 -0.233095 N 1.969517 -1.823272 -0.249881 C -2.835349 -0.204976 -0.611626 C -0.716010 0.646673 -0.098167 C -1.487863 0.469092 1.225915 C -2.933768 0.535203 0.727245 O -1.563487 0.196496 -1.148275 H -0.137410 -2.127283 -0.286449 H -2.838695 -1.285640 -0.429609 H -0.455489 1.693543 -0.257119 H -1.238287 1.264770 1.931583 H -3.216109 1.580429 0.555166 N 4.994090 -1.298929 -0.174277 H 4.731808 -2.271834 -0.233544 H 5.976774 -1.072529 -0.135357 H 3.815818 2.955485 0.077599 H 5.327643 1.231390 -0.003803 O -1.208264 -0.803936 1.782803 H -2.023678 -1.107156 2.208524 O -3.798043 -0.078650 1.664698 H -4.635368 -0.243987 1.206749 C -3.942663 0.154834 -1.581780 H -3.834951 -0.397292 -2.519951 H -3.915076 1.228845 -1.792402 O -5.154985 -0.207620 -0.905598 H -5.909998 0.097986 -1.418907	**Adenosine (Ref_aH^+)** N 4.310146 0.984815 -0.091587 C 3.359571 1.959595 -0.212574 N 2.081417 1.726371 -0.275055 C 1.775014 0.422147 -0.219856 C 2.664413 -0.638965 -0.109223 C 4.045892 -0.356835 -0.026304 N 0.507280 -0.121477 -0.269283 C 0.615432 -1.455829 -0.185973 N 1.898726 -1.792597 -0.096634 C -2.884912 -0.297134 -0.537217 C -0.757127 0.638765 -0.305191 C -1.435039 0.674029 1.081636 C -2.910631 0.645519 0.672432 O -1.638332 0.004866 -1.201196 H -0.207455 -2.148250 -0.206385 H -2.875379 -1.335941 -0.191938 H -0.491216 1.633828 -0.659952 H -1.151860 1.569831 1.637137 H -3.224642 1.647897 0.359685 N 5.027891 -1.223534 0.106076 H 4.857988 -2.216346 0.166002 H 5.993586 -0.928225 0.154942 H 3.738138 2.971823 -0.251935 H 5.278081 1.290617 -0.045010 O -1.089862 -0.499153 1.796229 H -1.868793 -0.759325 2.310612 O -3.694069 0.174561 1.749873 H -4.563196 -0.052718 1.387760 C -4.041521 -0.081288 -1.492014 H -3.989396 -0.777860 -2.333577 H -4.020049 0.944940 -1.872345 O -5.211060 -0.315056 -0.696798 H -5.995068 -0.084558 -1.205891 H 2.221064 -2.752535 -0.042885
Oxocarbenium ($R^{+\bullet}$) C 1.155778 -0.471567 -0.098505 C -1.119039 -0.428817 0.042565 C -0.767809 0.987285 -0.089050 C 0.761398 0.986600 0.120870 O -0.151724 -1.224709 0.055539 H 1.817151 -0.906874 0.643117 H 1.481286 -0.717193 -1.106575 H -2.113846 -0.861465 0.106772 H -1.343999 1.603853 0.604271 H -1.080023 1.294519 -1.098838 H 1.270111 1.640824 -0.583031 H 1.001143 1.303003 1.134686	

GR' N 2.613248 1.053532 -0.005938 C 1.399889 1.696439 -0.034425 N 0.249843 1.056312 -0.047087 C 0.381728 -0.287963 -0.038547 C 1.559548 -1.034804 -0.001077 C 2.811556 -0.348068 0.016600 N -0.636610 -1.214176 -0.047720 C -0.028664 -2.456981 -0.002433 N 1.278819 -2.390871 0.019602 O 3.953515 -0.802830 0.045827	**AR'** N -3.346278 1.023315 0.062430 C -2.365214 1.936384 0.012713 N -1.048053 1.734081 -0.059691 C -0.743699 0.429962 -0.077965 C -1.653420 -0.628670 -0.028786 C -3.017488 -0.283614 0.040710 N 0.502140 -0.159839 -0.152266 C 0.281174 -1.523750 -0.124967 N -0.989794 -1.844632 -0.055710 C 3.681109 -0.290137 0.959365

N 1.418050 3.053870 -0.097812 C -3.000325 0.969070 0.872920 C -2.081866 -0.976914 -0.050292 C -2.556243 -0.081621 -1.212113 C -3.561666 0.864428 -0.540952 O -2.488379 -0.353391 1.159352 H 3.464729 1.601655 -0.015813 H -0.616491 -3.362343 0.006090 H 0.533460 3.511029 0.064982 H 2.235643 3.558053 0.210711 H -2.180833 1.690987 0.925363 H -2.531530 -1.970024 -0.085443 H -2.991136 -0.680122 -2.011724 H -4.560143 0.421059 -0.519928 H -3.622770 1.832953 -1.038796 H -1.713667 0.477349 -1.616691 H -3.745543 1.196976 1.634395	C 1.779207 0.548867 -0.129421 C 2.773925 0.067656 -1.200590 C 4.114777 0.070785 -0.456901 O 2.414605 0.382487 1.137194 H 1.095721 -2.230496 -0.154377 H 3.544818 -1.371509 1.076256 H 1.519759 1.600777 -0.243419 H 2.755123 0.718540 -2.073690 H 4.564603 1.066281 -0.471142 N -4.001918 -1.206836 0.064636 H -3.775197 -2.181525 0.178305 H -4.948937 -0.908939 0.238034 H -2.689378 2.972134 0.035154 H 2.519901 -0.941103 -1.530423 H 4.829670 -0.640235 -0.872022 H 4.352175 0.068641 1.739029

E'-Q(H)	**Eq'-Q(H)**	**Eqn'-Q(H)**
C 2.112271 1.601495 0.372306 C 2.681012 0.281430 0.133477 C 1.676804 -0.888524 -0.130202 C 0.239710 -0.589507 -0.169396 C -0.178399 0.681015 0.063238 C 0.777534 1.763842 0.331326 O 3.876885 0.049070 0.129145 O 2.126014 -2.010647 -0.290201 C -0.698738 -1.736140 -0.427605 C -2.126829 -1.274049 -0.725025 C -2.568554 -0.145006 0.217596 C -1.637871 1.072143 0.050021 C -1.950970 1.885875 -1.222715 C -2.624137 -0.604795 1.679770 H 2.791506 2.419948 0.577126 H -0.680497 -2.399306 0.445687 H -0.309355 -2.337210 -1.253471 H -2.812627 -2.121105 -0.641009 H -2.185041 -0.925742 -1.760235 H -3.575451 0.169686 -0.074733 H -1.793820 1.741947 0.905014 H -2.980357 2.249557 -1.185497 H -1.830812 1.272530 -2.118276 H -1.290650 2.750709 -1.320541 H -3.027757 0.185906 2.317810 H -1.632410 -0.862833 2.061337 H -3.263527 -1.485463 1.786038 H 0.356599 2.747314 0.512463	C 2.099433 -1.658925 -0.353374 C 2.738224 -0.364118 -0.144910 C 1.799155 0.864317 0.092154 C 0.348875 0.648236 0.071252 C -0.134965 -0.602320 -0.118238 C 0.757458 -1.748108 -0.334628 O 3.944296 -0.196191 -0.151731 O 2.306034 1.955066 0.289682 C -0.543511 1.840558 0.260476 C -1.971652 1.557716 -0.103273 C -2.468388 0.332506 -0.281792 C -1.612244 -0.899205 -0.073894 C -1.951839 -1.598081 1.267668 C -3.897602 0.086857 -0.678585 H 2.736303 -2.518279 -0.523489 H -0.157914 2.672772 -0.338049 H -0.471743 2.190698 1.300076 H -2.617570 2.421302 -0.232590 H -1.832031 -1.616248 -0.875423 H -3.004882 -1.882192 1.294943 H -1.749633 -0.922484 2.101710 H -1.356323 -2.503725 1.403674 H -3.946088 -0.463108 -1.625028 H -4.442086 1.025086 -0.797454 H -4.423250 -0.519982 0.065372 H 0.284908 -2.711449 -0.494476	C -1.996769 1.689498 0.000862 C -2.703853 0.420599 -0.001382 C -1.839387 -0.874781 0.001413 C -0.372398 -0.723388 0.000384 C 0.216708 0.562826 0.000805 C -0.647836 1.738898 0.001763 O -3.920535 0.321151 -0.005127 O -2.404803 -1.953105 0.004497 C 0.433730 -1.857723 -0.000656 C 1.815334 -1.721640 -0.001329 C 2.423011 -0.462900 -0.000785 C 1.618302 0.700541 0.000327 C 2.251630 2.071931 0.000855 C 3.927348 -0.382179 -0.001329 H -2.595208 2.592601 0.001125 H -0.028351 -2.836526 -0.000980 H 2.439373 -2.607468 -0.002317 H 3.336440 2.015256 0.003026 H 1.952160 2.646088 0.881471 H 1.955548 2.645060 -0.881616 H 4.298302 0.151330 -0.880809 H 4.363916 -1.380884 -0.002838 H 4.298891 0.148826 0.879449 H -0.173274 2.711257 0.002955
E'-Q(H)H^+	**Eq'-Q(H)H^+**	**Eqn'-Q(H)H^+**
C 2.080048 1.624709 0.369944 C 2.583409 0.349545 0.150633 C 1.637575 -0.830898 -0.149646 C 0.191401 -0.582594 -0.178745 C -0.240208 0.685418 0.051269 C 0.713781 1.757991 0.308374 O 3.835635 0.070022 0.176293 O 2.178369 -1.899817 -0.342087 C -0.717095 -1.744536 -0.424772 C -2.157374 -1.307824 -0.703263 C -2.604972 -0.175687 0.234628 C -1.701764 1.059294 0.043777 C -2.030977 1.852061 -1.237785 C -2.633894 -0.620548 1.702475 H 2.736084 2.458095 0.578376 H 3.956302 -0.890685 -0.006375 H -0.667979 -2.399494 0.454313 H -0.320637 -2.342159 -1.250181 H -2.823068 -2.166745 -0.596004 H -2.236835 -0.975724 -1.741698 H -3.619417 0.117911 -0.049950 H -1.861153 1.734493 0.893246	C 2.077573 -1.666604 -0.366373 C 2.641174 -0.415354 -0.143423 C 1.750573 0.823581 0.083255 C 0.296181 0.644677 0.080042 C -0.193150 -0.603139 -0.120910 C 0.706272 -1.729040 -0.350844 O 3.905791 -0.206530 -0.119826 O 2.339107 1.871054 0.249402 C -0.574480 1.840705 0.281854 C -2.004238 1.569083 -0.088678 C -2.510115 0.349525 -0.277378 C -1.669277 -0.895721 -0.075177 C -2.007744 -1.596290 1.265268 C -3.938715 0.118673 -0.681932 H 2.696133 -2.535529 -0.541882 H 4.074017 0.749490 0.050591 H -0.175248 2.676916 -0.301842 H -0.495228 2.167447 1.328911 H -2.638476 2.440600 -0.213390 H -1.894094 -1.604869 -0.881026 H -3.061723 -1.875159 1.289219 H -1.801167 -0.925157 2.101323	C -1.970938 1.703780 0.000047 C -2.599149 0.473156 -0.000030 C -1.800948 -0.820754 0.000007 C -0.344673 -0.707912 -0.000024 C 0.261598 0.581357 0.000017 C -0.585811 1.734354 0.000096 O -3.885963 0.335430 -0.000097 O -2.451306 -1.852655 0.000107 C 0.433677 -1.848408 -0.000055 C 1.829523 -1.732285 -0.000041 C 2.456690 -0.495390 0.000015 C 1.670332 0.696616 0.000002 C 2.394293 2.008146 -0.000083 C 3.955334 -0.418988 0.000054 H -2.550721 2.616476 0.000086 H -4.090541 -0.627053 -0.000077 H -0.038154 -2.822362 -0.000092 H 2.433147 -2.631297 -0.000060 H 3.044114 2.074259 0.876998 H 1.745683 2.877751 -0.000206 H 3.044166 2.074109 -0.877135 H 4.321914 0.118879 -0.878729

H -3.063718 2.203304 -1.194665 H -1.908640 1.227751 -2.125103 H -1.382983 2.724447 -1.353167 H -3.044163 0.169634 2.336180 H -1.634425 -0.857668 2.077838 H -3.256270 -1.510807 1.823817 H 0.295282 2.744420 0.478386	H -1.418080 -2.506657 1.397750 H -3.985985 -0.420682 -1.634156 H -4.475022 1.062100 -0.792539 H -4.470055 -0.492133 0.054233 H 0.241417 -2.693130 -0.528024	H 4.392972 -1.416190 0.000263 H 4.321852 0.119249 0.878629 H -0.125844 2.711950 0.000214
E'-Q(H)-GR'(TS)	**Eq'-Q(H)-GR'(TS)**	**Eqn'-Q(H)-GR'(TS)**
C -2.414308 -3.061582 0.654159 C -2.046653 -1.943423 -0.344405 H -2.370793 -4.033594 0.159073 H -3.432125 -2.917150 1.027111 H -1.729768 -3.098576 1.501191 C -2.206106 -0.585081 0.306697 C -2.854125 -2.107099 -1.653249 H -0.982499 -2.056288 -0.590350 C -3.004486 -0.775810 -2.389122 C -3.003323 0.386083 -0.183294 H -3.863214 -2.439433 -1.375291 C -1.386251 -0.321996 1.532546 C -2.226775 -3.172422 -2.556105 C -3.705208 0.253969 -1.508523 H -2.012359 -0.400453 -2.669875 C -1.661952 0.800006 2.352224 H -3.564446 -0.925264 -3.316806 C -3.178846 1.655264 0.561850 H -1.054989 -1.214250 2.048971 H -1.235787 -2.850814 -2.893291 H -2.844575 -3.341927 -3.442102 H -2.111339 -4.129967 -2.042833 C -2.510441 1.830390 1.945455 H -4.753480 -0.030658 -1.352369 H -3.729711 1.234586 -1.988714 H -1.168741 0.876626 3.314958 O -3.860188 2.561025 0.100300 O -2.800592 2.859181 2.602348 N 0.250558 -0.108365 0.689006 C 0.555452 0.953856 -0.023626 C 1.342410 -0.954172 0.662188 N 1.818417 0.852695 -0.524786 H -0.094804 1.790843 -0.210308 C 1.586864 -2.223696 1.267720 C 2.338218 -0.353726 -0.102403 N 3.564745 -0.828665 -0.379039 O 0.849824 -2.894151 1.982187 N 2.883519 -2.677334 0.937951 C 3.805817 -2.008193 0.166197 H 3.133370 -3.570857 1.345291 N 5.013519 -2.585325 0.002384 H 5.167434 -3.554503 0.230971 H 5.639292 -2.162188 -0.665164 C 2.526967 1.867467 -1.357313 C 3.577731 2.616205 -0.538177 H 2.929822 1.330234 -2.214783 C 1.761101 4.064432 -1.043636 C 2.744937 3.746386 0.079549 H 4.329231 3.013658 -1.223715 H 4.074120 1.974707 0.187669 H 2.158808 4.806695 -1.739259 H 0.779096 4.385191 -0.696085 H 3.346653 4.611296 0.356745 H 2.218928 3.396092 0.970605 O 1.587260 2.815670 -1.781416	C 3.001979 -2.818124 -0.757778 C 2.136185 -1.911627 0.152963 H 2.887660 -3.865816 -0.473327 H 4.055835 -2.545317 -0.668815 H 2.703904 -2.722146 -1.804101 C 2.246225 -0.483959 -0.315566 C 2.520497 -2.075899 1.608414 C 3.286674 -1.171655 2.220987 C 3.037151 0.412761 0.299861 C 1.443806 -0.095670 -1.514315 C 2.005300 -3.310263 2.294308 C 3.782574 0.083973 1.563817 C 1.698634 1.134822 -2.166252 C 3.178330 1.778831 -0.249276 H 1.165994 -0.933493 -2.145263 H 0.909532 -3.325232 2.286820 H 2.343587 -3.360700 3.330814 H 2.335065 -4.220597 1.783197 C 2.507604 2.125285 -1.602262 H 3.699058 0.930915 2.252488 H 1.219949 1.331473 -3.119074 O 3.831248 2.627948 0.341792 O 2.767203 3.244483 -2.103744 N -0.222015 -0.039015 -0.701640 C -0.620329 1.008173 -0.013454 C -1.237659 -0.975558 -0.657519 N -1.870077 0.808573 0.490273 H -0.045335 1.903894 0.146318 C -1.375314 -2.268965 -1.245373 C -2.282936 -0.447123 0.094089 N -3.464321 -1.020298 0.380708 O -0.582087 -2.885715 -1.948128 N -2.629929 -2.823880 -0.909982 C -3.603660 -2.225499 -0.143563 H -2.805931 -3.739283 -1.306983 N -4.754535 -2.904977 0.036768 H -4.818235 -3.889580 -0.168469 H -5.412549 -2.527808 0.700953 C -2.670411 1.780971 1.289986 C -3.774598 2.412537 0.442812 H -3.032437 1.234859 2.159851 C -2.090734 4.024408 0.913274 C -3.035752 3.590403 -0.204556 H -4.562704 2.764771 1.111803 H -4.208747 1.709772 -0.266008 H -2.553790 4.752839 1.582466 H -1.135916 4.414140 0.560535 H -3.706319 4.392603 -0.510755 H -2.475495 3.259650 -1.082089 O -1.820162 2.818497 1.692302 H 1.099870 -2.238967 0.028359 H 4.858305 0.007692 1.349467 H 3.573823 -1.325120 3.257575	C -1.830346 -1.862392 -2.464932 C -2.586760 -1.039804 -1.452687 H -1.514750 -1.236299 -3.304119 H -2.466810 -2.649992 -2.879378 H -0.939202 -2.331051 -2.058014 C -2.210324 -0.970156 -0.102068 C -3.707675 -0.298680 -1.891719 C -4.398717 0.510636 -0.987710 C -2.910632 -0.136015 0.790140 C -1.029918 -1.713697 0.419244 C -4.156574 -0.366135 -3.326392 C -4.003401 0.601808 0.339217 C -0.828302 -1.833286 1.821482 C -2.504305 -0.030570 2.216846 H -0.763619 -2.597917 -0.143178 H -3.375296 -0.007922 -4.003878 H -5.047831 0.241569 -3.483797 H -4.385145 -1.393675 -3.624291 C -1.464186 -1.022943 2.764375 H -0.085921 -2.543595 2.167054 O -2.993789 0.814145 2.952629 O -1.285656 -1.052952 4.006764 N 0.334745 -0.699232 -0.286864 C 0.278090 0.597513 -0.517184 C 1.670949 -1.050664 -0.246871 N 1.530636 1.123140 -0.637463 H -0.621187 1.181380 -0.600139 C 2.322394 -2.306535 -0.058049 C 2.431832 0.092053 -0.472153 N 3.770799 0.193356 -0.533261 O 1.831621 -3.413635 0.130597 N 3.725327 -2.138901 -0.116284 C 4.392826 -0.957085 -0.340687 H 4.257621 -2.990021 0.021930 N 5.740523 -0.992405 -0.328701 H 6.244780 -1.863487 -0.372463 H 6.227010 -0.158644 -0.618938 C 1.868132 2.558068 -0.866476 C 2.411874 3.199740 0.409290 H 2.556639 2.583443 -1.709815 C 0.227851 4.025235 -0.049206 C 1.119151 3.616707 1.121785 H 3.004395 4.073279 0.128923 H 3.041687 2.521052 0.981430 H 0.346941 5.079411 -0.308201 H -0.829561 3.808518 0.103082 H 1.270541 4.433010 1.827224 H 0.687908 2.772248 1.664122 O 0.687302 3.237494 -1.191205 H -5.254947 1.078131 -1.334459 H -4.535026 1.235671 1.037168
E'-Q(H)-AR'(TS)	**Eq'-Q(H)-AR'(TS)**	**Eqn'-Q(H)-AR'(TS)**
N -0.696594 3.290915 -0.403903 C -0.033487 2.218505 -0.016733 N -0.508963 0.972314 0.116925 C -1.823416 0.826283 -0.172611 C -2.619878 1.905232 -0.565892 C -2.017108 3.173864 -0.686431	N -0.463810 3.288368 -0.406275 C 0.112432 2.217296 0.106196 N -0.417724 0.994547 0.239580 C -1.696427 0.871462 -0.187714 C -2.396453 1.946534 -0.743208 C -1.738797 3.189232 -0.854122	N 0.021405 2.991203 -1.058267 C 0.486293 1.808384 -0.714570 N -0.227512 0.703832 -0.414784 C -1.575865 0.861091 -0.500230 C -2.161508 2.091094 -0.803110 C -1.319865 3.184959 -1.091007

N -2.653428 -0.272977 -0.188170	N -2.571491 -0.191748 -0.209987	N -2.620449 -0.023156 -0.348088
C -3.898131 0.204188 -0.576341	C -3.738940 0.296951 -0.779123	C -3.772499 0.731049 -0.526956
N -3.912078 1.490154 -0.810942	N -3.668469 1.560591 -1.108754	N -3.535913 1.986581 -0.805182
C -2.593191 -2.963572 2.056931	C -2.786035 -2.484665 2.403523	C -3.428237 -2.478687 1.809083
C -2.287422 -1.655905 0.126310	C -2.327369 -1.547810 0.295596	C -2.521885 -1.473712 -0.094373
C -3.353225 -2.706642 -0.175242	C -3.497238 -2.518901 0.143776	C -3.750748 -2.290653 -0.531709
C -2.983239 -3.795840 0.838012	C -3.257700 -3.460151 1.329957	C -3.910919 -3.295757 0.618057
O -2.000193 -1.752668 1.516651	O -2.036738 -1.469281 1.685286	O -2.315785 -1.715621 1.285716
H -4.744114 -0.452623 -0.681954	H -4.594776 -0.336385 -0.937023	H -4.753122 0.296389 -0.440890
H -1.852022 -3.438934 2.698640	H -2.118642 -2.925446 3.143120	H -3.049548 -3.070569 2.640779
H -3.465273 -2.685007 2.655175	H -3.626018 -2.004010 2.913282	H -4.202800 -1.794923 2.173168
H -1.379616 -1.867195 -0.443405	H -1.447302 -1.923688 -0.231921	H -1.637995 -1.799986 -0.637481
H -3.323343 -3.032111 -1.213951	H -3.496740 -3.012742 -0.826679	H -3.579604 -2.755511 -1.501158
H -4.351234 -2.329658 0.050700	H -4.449765 -2.005719 0.281624	H -4.643856 -1.674882 -0.611234
H -3.810456 -4.474767 1.043348	H -4.157630 -4.000873 1.621821	H -4.939166 -3.639974 0.729756
H -2.132069 -4.381320 0.482811	H -2.474452 -4.185312 1.097850	H -3.264708 -4.163719 0.470015
N -2.691552 4.260155 -1.069509	N -2.322020 4.268075 -1.380877	N -1.787840 4.394875 -1.399026
H -3.674381 4.206415 -1.285613	H -3.269270 4.226057 -1.722197	H -2.779859 4.570806 -1.428595
H -2.216511 5.146400 -1.143742	H -1.813230 5.136614 -1.439454	H -1.146250 5.146021 -1.601732
C 1.014535 0.336591 2.153351	C 1.163181 0.281706 2.231768	C 0.453108 -0.059213 1.962336
C 2.243354 0.942387 2.388428	C 2.445221 0.786472 2.433406	C 1.480233 0.540272 2.681470
C 0.641296 -0.194226 0.879006	C 0.715332 -0.228520 0.976740	C 0.565471 -0.487923 0.591019
C 3.229330 0.936525 1.203399	C 3.402328 0.701048 1.226564	C 2.833425 0.647651 1.969124
O 2.636281 1.454936 3.468754	O 2.906842 1.257655 3.503821	O 1.407057 0.967344 3.866822
C 1.679779 -0.381623 -0.184620	C 1.700928 -0.446505 -0.125920	C 1.928595 -0.634948 -0.005269
C 2.904217 0.160686 -0.024459	C 2.977426 -0.044501 0.018570	C 3.018213 -0.063102 0.672856
O 4.288497 1.542481 1.286209	O 4.503824 1.230332 1.275155	O 3.749342 1.287268 2.467744
C 1.335379 -1.249830 -1.382021	C 1.264849 -1.159553 -1.389917	C 2.114565 -1.307513 -1.224775
C 4.036892 -0.028865 -0.998480	C 4.022889 -0.361944 -1.016425	C 4.298953 -0.170244 0.132258
C 2.610902 -1.875409 -1.989261	C 2.400621 -1.994602 -1.959843	C 3.417225 -1.414861 -1.757646
C 0.519866 -0.504269 -2.459791	C 0.776987 -0.180019 -2.488315	C 0.935193 -1.905962 -1.951214
H 0.714624 -2.074481 -1.011544	H 0.434016 -1.828442 -1.144857	C 4.488877 -0.839903 -1.066709
C 3.633291 -0.768370 -2.276236	C 3.660650 -1.583989 -1.814999	H 5.133170 0.269323 0.663483
H 4.834572 -0.570018 -0.475937	H 4.986381 -0.497566 -0.519355	C 3.686658 -2.136745 -3.053679
H 4.467110 0.947215 -1.237550	H 4.165270 0.504508 -1.678529	H 0.445599 -2.673055 -1.344054
C 3.184074 -2.979954 -1.093891	C 2.006752 -3.228433 -2.719251	H 1.228100 -2.376290 -2.885808
H 2.323502 -2.332721 -2.941407	H -0.143680 0.330562 -2.210472	H 0.190152 -1.142851 -2.189099
H 0.410224 -1.143603 -3.339021	H 0.584827 -0.727380 -3.413176	H 5.487486 -0.925189 -1.479994
H 1.016400 0.418632 -2.765248	H 1.543637 0.571303 -2.687805	H 3.372489 -3.182974 -3.003181
H -0.480512 -0.242023 -2.120873	H 4.473757 -2.142199 -2.269105	H 4.751222 -2.116213 -3.287977
H 4.522010 -1.191249 -2.752551	H 1.499972 -3.941439 -2.059365	H 3.148981 -1.677712 -3.888065
H 3.205346 -0.059786 -2.990388	H 2.876369 -3.721750 -3.157046	H 1.560138 1.696175 -0.645102
H 2.456769 -3.785902 -0.962434	H 1.303889 -2.992524 -3.525393	H -0.516742 -0.170168 2.432667
H 3.445996 -2.605184 -0.101216	H 1.127444 2.319407 0.470338	H -0.068132 -1.331615 0.359930
H 4.086406 -3.408183 -1.539206	H 0.463142 0.281414 3.059932	
H 1.012609 2.342056 0.233051	H -0.017846 -1.019500 1.060976	
H 0.284135 0.295721 2.954184		
H -0.051471 -1.022121 0.943855		
E'-Q(H)-GR'	**Eq'-Q(H)-GR'**	**Eqn'-Q(H)-GR'**
C -2.030955 -0.493611 -2.310083	C -1.983721 -1.143871 -2.067100	C 1.693589 -2.169503 -0.767248
C -3.059090 -1.391178 -2.128109	C -3.041133 -1.961826 -1.737279	C 2.597717 -2.041501 -1.799916
C -3.688390 -1.406775 -0.736837	C -3.787183 -1.605515 -0.453442	C 3.487953 -0.807808 -1.761157
C -3.299494 -0.386872 0.273512	C -3.377505 -0.417044 0.337577	C 3.443228 0.090730 -0.570858
C -2.304929 0.486678 0.033881	C -2.351470 0.360864 -0.041693	C 2.503895 -0.084290 0.457229
C -1.540176 0.438881 -1.270043	C -1.544715 0.028802 -1.274114	C 1.486745 -1.190444 0.327745
O -3.522434 -2.201302 -2.996849	O -3.451572 -2.971517 -2.398736	O 2.758495 -2.859177 -2.764081
O -4.525071 -2.257455 -0.444694	O -4.732604 -2.290936 -0.072044	O 4.249448 -0.559212 -2.690298
C -4.037481 -0.443892 1.588096	C -4.161123 -0.128466 1.591209	C 4.370735 1.131706 -0.481438
C -3.741837 0.739578 2.513056	C -3.446810 0.804573 2.524961	C 4.352397 1.987768 0.607417
C -2.263079 1.145515 2.469526	C -2.433255 1.586203 2.150386	C 3.419694 1.829822 1.637065
C -1.878666 1.542817 1.030846	C -1.979855 1.620176 0.705341	C 2.483773 0.777441 1.567673
C -2.437622 2.922088 0.627032	C -2.564438 2.857350 -0.022127	C 1.466699 0.631323 2.673352
C -1.340471 0.041997 3.001767	C -1.699816 2.491883 3.099364	C 3.424033 2.787649 2.799173
N 2.462115 2.761518 -0.869278	N 2.380065 2.501431 -1.416429	N -2.817120 -2.432462 1.382349
C 3.475327 1.967897 -0.382287	C 3.421542 1.857667 -0.788656	C -3.756537 -1.542547 0.914735
N 3.310519 0.683272 -0.107519	N 3.295177 0.661237 -0.236027	N -3.434322 -0.431111 0.270605
C 2.068112 0.239742 -0.332556	C 2.062315 0.149955 -0.333336	C -2.115857 -0.263452 0.113296
C 0.986282 0.965473 -0.811195	C 0.954025 0.728884 -0.935036	C -1.101635 -1.107807 0.541855
C 1.141532 2.349583 -1.139068	C 1.067097 2.010211 -1.561434	C -1.418409 -2.305580 1.255708
N 1.608799 -1.056844 -0.137111	N 1.644092 -1.087218 0.141557	N -1.490156 0.808122 -0.509381
C 0.308165 -1.098137 -0.499225	C 0.341747 -1.240093 -0.181756	C -0.154428 0.598676 -0.457984

N -0.093836 0.098314 -0.900923 O 0.314026 3.131212 -1.587812 N 4.669480 2.541845 -0.171408 C 4.700142 -2.332061 0.092216 C 2.380851 -2.227145 0.349667 C 3.011236 -1.986465 1.733719 C 4.422548 -2.569892 1.572237 O 3.415034 -2.528600 -0.554044 H -1.526248 -0.450721 -3.270490 H -1.441614 1.454325 -1.660649 H -3.770065 -1.388750 2.075772 H -5.110427 -0.519258 1.394459 H -4.032078 0.487313 3.536991 H -4.356976 1.594279 2.218062 H -2.129363 2.030120 3.101156 H -0.787103 1.623666 0.998246 H -2.092544 3.682400 1.332766 H -3.529474 2.922012 0.626056 H -2.094720 3.211114 -0.367793 H -0.300698 0.380761 3.016044 H -1.385704 -0.857349 2.381453 H -1.618700 -0.241216 4.020682 H 2.648420 3.736889 -1.072330 H -0.316116 -1.974601 -0.464026 H 5.433425 1.954659 0.123458 H 4.870083 3.490221 -0.444363 H 5.391083 -3.045281 -0.354580 H 5.039347 -1.311219 -0.097117 H 1.661896 -3.046507 0.350445 H 2.426846 -2.468746 2.515741 H 3.056604 -0.918961 1.944889 H 5.152020 -2.078403 2.216455 H 4.428093 -3.639660 1.792631	N -0.100737 -0.166771 -0.820222 O 0.212144 2.654542 -2.153988 N 4.602470 2.492933 -0.726894 C 4.774675 -2.233491 0.491958 C 2.465099 -2.117710 0.825445 C 3.143350 -1.587510 2.101615 C 4.562283 -2.166496 2.000018 O 3.470362 -2.579186 -0.043284 H -1.418287 -1.348325 -2.971280 H -1.469579 0.925759 -1.894772 H -4.379414 -1.075086 2.094081 H -5.148134 0.274606 1.322277 H -3.784270 0.818080 3.557696 H -0.889645 1.729169 0.697039 H -2.284432 3.773974 0.501125 H -3.654432 2.793504 -0.051048 H -2.184399 2.927448 -1.042520 H -0.638197 2.223629 3.145229 H -2.113824 2.431480 4.107520 H -1.745673 3.536205 2.773512 H 2.536090 3.412761 -1.831706 H -0.255270 -2.107412 0.043418 H 5.388494 1.989135 -0.347250 H 4.782917 3.344814 -1.233177 H 5.464726 -3.012259 0.170851 H 5.081623 -1.268470 0.082604 H 1.769788 -2.933172 1.025158 H 2.604112 -1.910523 2.990704 H 3.168533 -0.498838 2.088507 H 5.303687 -1.540409 2.496990 H 4.604834 -3.167851 2.434153	N 0.107703 -0.535388 0.173850 O -0.661324 -3.145749 1.722378 N -5.048895 -1.835887 1.120218 C -4.312573 1.861659 -1.978149 C -2.131665 1.983615 -1.148959 C -3.038631 2.767010 -0.182297 C -4.278107 3.062469 -1.039657 O -2.915848 1.564281 -2.238701 H 1.034023 -3.031652 -0.757469 H 1.386219 -1.715453 1.278237 H 5.070922 2.797726 0.666980 H 0.657769 1.361121 2.557917 H 1.922189 0.812259 3.647818 H 1.012283 -0.356826 2.705243 H 2.450426 3.270892 2.921670 H 4.175230 3.564922 2.656489 H 3.644062 2.273762 3.740109 H -3.122637 -3.264357 1.874143 H 0.586007 1.261907 -0.870947 H -5.742434 -1.168067 0.823338 H -5.346417 -2.633926 1.657149 H -4.778934 2.059438 -2.942074 H -4.778082 0.993038 -1.507152 H -1.299367 2.580295 -1.522505 H -2.537065 3.662580 0.181053 H -3.299966 2.145859 0.673299 H -5.186011 3.149709 -0.442320 H -4.145679 3.985420 -1.608547 H 5.095119 1.255690 -1.275804
E'-Q(H)-AR'	**Eq'-Q(H)-AR'**	**Eqn'-Q(H)-AR'**
N -0.861935 3.232024 0.492070 C -0.122981 2.179815 0.728178 N -0.454457 0.885299 0.489109 C -1.693437 0.676342 -0.040525 C -2.538127 1.753856 -0.322010 C -2.098541 3.064270 -0.046678 N -2.387451 -0.452479 -0.406959 C -3.608330 0.007708 -0.885180 N -3.728029 1.308020 -0.852221 C -2.907661 -2.743742 1.783138 C -1.991067 -1.879239 -0.203633 C -3.079858 -2.868813 -0.602725 C -3.938920 -2.947770 0.667700 O -1.752931 -2.102346 1.160583 H -4.360536 -0.671532 -1.246942 H -2.556464 -3.686884 2.203946 H -3.263974 -2.099763 2.587041 H -1.063595 -2.028670 -0.751481 H -2.580710 -3.821536 -0.786351 H -3.620736 -2.605810 -1.509007 H -4.692247 -2.158363 0.685590 H -4.452611 -3.904043 0.757142 N -2.840387 4.140222 -0.289444 H -3.761215 4.050701 -0.690713 H -2.481265 5.058269 -0.074798 C 1.080958 -0.032133 2.174678 C 2.395448 0.073816 2.569562 C 0.633478 -0.160379 0.767266 C 3.424000 0.069229 1.444883 O 2.820804 0.157455 3.768465 C 1.684809 -0.078381 -0.311030 C 2.988175 -0.034825 0.025701 O 4.623732 0.142573 1.701736 C 1.231312 -0.166346 -1.758521 C 4.103325 -0.159142 -0.983801 C 2.290377 -0.903247 -2.607578 C 0.905689 1.218494 -2.360390	N 0.433397 3.322103 0.694786 C -0.227321 2.366411 0.097052 N 0.269159 1.166632 -0.297565 C 1.600013 0.970238 -0.080639 C 2.367005 1.937477 0.577802 C 1.752918 3.142323 0.974505 N 2.464175 -0.045585 -0.393859 C 3.699488 0.351950 0.100373 N 3.675085 1.522280 0.683703 C 3.938736 -2.937480 -1.207786 C 2.266814 -1.298443 -1.186057 C 1.783664 -2.485274 -0.328545 C 2.646164 -3.648241 -0.835773 O 3.507452 -1.657366 -1.740571 H 4.567503 -0.270805 -0.030845 H 4.516017 -3.426975 -1.989802 H 4.578704 -2.771412 -0.334937 H 1.591901 -1.041381 -2.001699 H 0.716787 -2.669062 -0.443753 H 1.987956 -2.281188 0.723898 H 2.792352 -4.418592 -0.078901 H 2.197179 -4.106267 -1.719460 N 2.407582 4.114222 1.601990 H 3.387474 4.017741 1.819877 H 1.925533 4.963184 1.856372 C -1.298097 0.694169 -2.141428 C -2.647311 0.822445 -2.392682 C -0.725018 0.158812 -0.884462 C -3.580430 0.381455 -1.267690 O -3.178115 1.264163 -3.461862 C -1.691885 -0.261011 0.190929 C -3.015463 -0.222360 -0.034746 O -4.796081 0.515591 -1.376843 C -1.134847 -0.815209 1.487150 C -3.983203 -0.818681 0.954314 C -2.025569 -1.920901 2.028276 C -0.972952 0.275933 2.576060	N -0.004716 3.077588 -0.901088 C -0.514794 1.885528 -0.723077 N 0.168088 0.751353 -0.432674 C 1.524196 0.877761 -0.364289 C 2.141253 2.120770 -0.532086 C 1.339794 3.247557 -0.804678 N 2.537978 -0.017682 -0.141464 C 3.707709 0.728955 -0.178512 N 3.506651 2.000814 -0.408204 C 4.483315 -2.596297 0.752361 C 2.524674 -1.491853 0.095396 C 2.389043 -1.858707 1.586486 C 3.407558 -2.993881 1.752672 O 3.751100 -2.012275 -0.356907 H 4.664758 0.254189 -0.046290 H 5.056652 -3.429457 0.350230 H 5.170591 -1.851610 1.167685 H 1.729979 -1.900328 -0.524978 H 1.374336 -2.159792 1.843446 H 2.659671 -0.998699 2.201766 H 3.787588 -3.067055 2.771479 H 2.966532 -3.953007 1.473800 N 1.842209 4.467507 -0.974640 H 2.835602 4.628614 -0.912244 H 1.227425 5.241778 -1.175006 C -0.612051 -1.249143 -1.657813 C -1.742735 -1.532413 -2.396730 C -0.580868 -0.597795 -0.328198 C -3.071261 -1.146700 -1.762145 O -1.767765 -2.077744 -3.544875 C -1.910405 -0.368757 0.352448 C -3.089498 -0.632962 -0.362548 O -4.118436 -1.264059 -2.388609 C -1.965533 0.110430 1.673331 C -4.326219 -0.414875 0.249137 C -3.222458 0.339972 2.269890 C -0.720508 0.424544 2.465665

H 0.311587 -0.759815 -1.796346 C 3.642032 -0.196579 -2.445172 H 4.657002 -1.071710 -0.734144 H 4.818551 0.652756 -0.830715 C 2.363330 -2.393420 -2.257878 H 1.981669 -0.818298 -3.654736 H 0.740142 1.120275 -3.436176 H 1.723484 1.923026 -2.201856 H 0.003533 1.656345 -1.934900 H 4.400241 -0.696379 -3.054471 H 3.560731 0.822761 -2.830715 H 1.398819 -2.879753 -2.429446 H 2.634063 -2.552428 -1.210990 H 3.110086 -2.897827 -2.877277 H 0.861542 2.311024 1.158475 H 0.299955 -0.080111 2.927250 H 0.120839 -1.112381 0.641549	H -0.142401 -1.232422 1.294839 C -3.339768 -1.876315 1.808028 H -4.834865 -1.231416 0.408457 H -4.409902 -0.022609 1.581311 C -1.350441 -2.986401 2.842929 H -0.692554 -0.185125 3.525090 H -1.913893 0.810734 2.718539 H -0.197119 0.999384 2.325631 H -3.990624 -2.630930 2.239605 H -0.632858 -3.543576 2.230429 H -2.074368 -3.692783 3.253145 H -0.783925 -2.554059 3.674587 H -1.279951 2.504911 -0.114674 H -0.585027 0.979993 -2.908278 H -0.110741 -0.719377 -1.084270	C -4.386508 0.069545 1.544794 C -3.328966 0.874637 3.673732 H -0.837695 0.130158 3.508928 H -0.509812 1.499333 2.456413 H 0.163085 -0.082620 2.088375 H -5.350275 0.244375 2.009774 H -2.907197 0.174203 4.401365 H -4.371185 1.050120 3.941325 H -2.783786 1.816085 3.785485 H -1.586757 1.766259 -0.800913 H 0.350581 -1.479617 -2.104874 H 0.043043 -1.157163 0.368071 H -5.228229 -0.628102 -0.309234
E'-Q(H)H$^+$-GR'	**Eq'-Q(H)H$^+$-GR'**	**Eqn'-Q(H)H$^+$-GR'**
C -1.902821 -0.324238 -2.269692 C -3.015318 -1.059659 -2.187768 C -3.818913 -1.115619 -0.939899 C -3.399127 -0.314394 0.217033 C -2.285603 0.444419 0.150682 C -1.449497 0.500845 -1.111815 O -3.490134 -1.807157 -3.204731 O -4.814058 -1.839863 -0.933548 C -4.247431 -0.437184 1.455874 C -3.889674 0.582972 2.539212 C -2.373754 0.793471 2.647382 C -1.820966 1.307554 1.302249 C -2.177669 2.786663 1.041735 C -1.640653 -0.474932 3.100697 N 2.524805 2.786443 -0.816645 C 3.553577 1.982134 -0.379840 N 3.393747 0.693325 -0.112941 C 2.144282 0.256962 -0.294274 C 1.051144 0.994075 -0.721178 C 1.194842 2.382142 -1.034446 N 1.683394 -1.040317 -0.091918 C 0.372380 -1.073804 -0.398270 N -0.037646 0.134551 -0.773391 O 0.344126 3.165685 -1.434057 N 4.756995 2.545452 -0.211834 C 4.772978 -2.329911 -0.061285 C 2.475070 -2.225426 0.338878 C 3.186543 -2.001680 1.685589 C 4.587071 -2.579430 1.430904 O 3.448670 -2.519839 -0.628032 H -1.306904 -0.291780 -3.173483 H -1.374751 1.545910 -1.427713 H -4.295573 -2.241320 -2.867623 H -4.133629 -1.459791 1.834071 H -5.300179 -0.348995 1.176749 H -4.291779 0.251919 3.500138 H -4.371750 1.537501 2.311921 H -2.187912 1.574079 3.391705 H -0.728720 1.250416 1.355593 H -1.815221 3.399545 1.870440 H -3.257175 2.923395 0.956194 H -1.712584 3.155443 0.126200 H -0.572286 -0.279678 3.227447 H -1.743719 -1.286694 2.375248 H -2.035948 -0.830307 4.055999 H 2.705756 3.764754 -1.011554 H -0.251857 -1.949318 -0.338694 H 5.526976 1.952914 0.056070 H 4.951032 3.499493 -0.469934 H 5.432176 -3.041147 -0.556267 H 5.101665 -1.308553 -0.264596 H 1.749563 -3.038056 0.372965 H 2.651436 -2.497693 2.493678	C -1.940885 -0.964046 -2.076300 C -3.076522 -1.627641 -1.838234 C -3.901474 -1.351497 -0.634059 C -3.452328 -0.320254 0.307025 C -2.326123 0.377366 0.071270 C -1.488061 0.125524 -1.162157 O -3.557385 -2.591870 -2.648913 O -4.930707 -2.007593 -0.479000 C -4.288827 -0.095972 1.535676 C -3.547996 0.650131 2.606293 C -2.436748 1.351957 2.381874 C -1.875601 1.493682 0.980877 C -2.262823 2.864029 0.366902 C -1.683106 2.064023 3.469373 N 2.453854 2.443704 -1.536110 C 3.501588 1.787269 -0.929343 N 3.362429 0.612650 -0.329687 C 2.115897 0.134234 -0.365718 C 1.006098 0.726907 -0.946359 C 1.124672 1.988765 -1.608382 N 1.674723 -1.069127 0.176722 C 0.358759 -1.190447 -0.081916 N -0.072767 -0.124489 -0.750653 O 0.253932 2.637766 -2.172604 N 4.705100 2.372673 -0.958511 C 4.785475 -2.277615 0.499594 C 2.489724 -2.094121 0.885161 C 3.211070 -1.524279 2.119684 C 4.613066 -2.141582 2.007974 O 3.458509 -2.612299 0.011776 H -1.333103 -1.171557 -2.948408 H -1.429419 1.059740 -1.730485 H -4.384852 -2.903924 -2.238556 H -4.628384 -1.065404 1.912380 H -5.209755 0.435085 1.256898 H -3.953983 0.590149 3.611588 H -0.782481 1.470894 1.052026 H -1.932687 3.673581 1.019955 H -3.346620 2.930074 0.251901 H -1.792400 3.009318 -0.607064 H -0.660384 1.678054 3.544798 H -2.171013 1.938653 4.437322 H -1.600763 3.136221 3.264724 H 2.620553 3.334477 -1.990526 H -0.253080 -2.025650 0.214896 H 5.476630 1.903222 -0.511543 H 4.866269 3.270364 -1.385468 H 5.446615 -3.087249 0.194970 H 5.104566 -1.339339 0.040904 H 1.778581 -2.881249 1.136011 H 2.687023 -1.795010 3.034803 H 3.261212 -0.438079 2.058073 H 5.380866 -1.512750 2.459069	C -1.734724 2.091494 -0.784596 C -2.753273 1.937826 -1.636495 C -3.683147 0.785512 -1.547432 C -3.498217 -0.171823 -0.448253 C -2.456972 -0.015847 0.484175 C -1.463975 1.113734 0.315114 O -3.013030 2.803021 -2.638227 O -4.571510 0.698528 -2.393106 C -4.394430 -1.235709 -0.321402 C -4.244610 -2.138680 0.715587 C -3.222441 -1.994105 1.660157 C -2.323330 -0.911369 1.556711 C -1.230385 -0.761351 2.585623 C -3.095902 -2.998743 2.773070 N 2.764663 2.380634 1.537777 C 3.730581 1.539631 1.031774 N 3.442977 0.477447 0.291920 C 2.134624 0.305962 0.082633 C 1.099761 1.101786 0.546619 C 1.375141 2.245210 1.358567 N 1.538804 -0.723406 -0.639154 C 0.203977 -0.538794 -0.611793 N -0.090889 0.541705 0.103417 O 0.582521 3.031642 1.859112 N 5.010447 1.827899 1.300565 C 4.420964 -1.629031 -2.088055 C 2.216420 -1.842771 -1.348282 C 3.100003 -2.686750 -0.411766 C 4.373708 -2.897469 -1.243981 O 3.027974 -1.330414 -2.372503 H -1.057799 2.932836 -0.872084 H -1.374760 1.669475 1.250343 H -4.931515 -2.971900 0.805916 H -0.377085 -1.407077 2.352253 H -1.587586 -1.049253 3.574106 H -0.860254 0.259661 2.662444 H -2.094969 -3.437863 2.799993 H -3.820883 -3.803429 2.651614 H -3.266825 -2.533523 3.748747 H 3.043322 3.177391 2.099152 H -0.516293 -1.179458 -1.091361 H 5.721387 1.194685 0.970178 H 5.282614 2.583740 1.907836 H 4.920182 -1.747859 -3.048311 H 4.857088 -0.791852 -1.538941 H 1.401843 -2.415410 -1.791801 H 2.599997 -3.614444 -0.138339 H 3.320478 -2.131836 0.499093 H 5.261257 -3.016123 -0.622169 H 4.277249 -3.776636 -1.884703 H -3.794360 2.452228 -3.103914 H -5.195369 -1.337790 -1.041776

H 3.242202 -0.937518 1.910024 H 5.353475 -2.090379 2.032528 H 4.609034 -3.650677 1.642335	H 4.643309 -3.124123 2.483926	
E'-Q(H)H^+-AR'	**Eq'-Q(H)H^+-AR'**	**Eqn'-Q(H)H^+-AR'**
N -0.986690 3.126508 0.868392 C -0.210499 2.084819 0.962629 N -0.502034 0.815158 0.559933 C -1.741972 0.632460 0.011165 C -2.617043 1.711332 -0.133964 C -2.220561 2.990063 0.309850 N -2.403525 -0.462031 -0.487167 C -3.638166 0.017997 -0.908304 N -3.794009 1.300365 -0.714985 C -2.727500 -2.916787 1.499348 C -1.956616 -1.891436 -0.469593 C -3.053738 -2.865907 -0.878113 C -3.823646 -3.063696 0.436224 O -1.608683 -2.243864 0.841034 H -4.371203 -0.633343 -1.351562 H -2.349815 -3.877015 1.850974 H -3.034947 -2.312709 2.352728 H -1.071576 -1.955530 -1.099268 H -2.551192 -3.788648 -1.171966 H -3.659120 -2.543690 -1.721954 H -4.591745 -2.298991 0.562295 H -4.308615 -4.037660 0.483114 N -2.994446 4.061803 0.208928 H -3.913674 3.996646 -0.201809 H -2.664977 4.954990 0.544263 C 1.022215 -0.287834 2.109335 C 2.318639 -0.273002 2.433678 C 0.595915 -0.207404 0.681702 C 3.371603 -0.129917 1.398422 O 2.771879 -0.393043 3.697394 C 1.670498 0.030996 -0.354011 C 2.975664 0.009193 -0.009242 O 4.545058 -0.142911 1.770204 H 3.744798 -0.360822 3.639423 C 1.232718 0.165506 -1.799793 C 4.105028 0.043841 -1.005851 C 2.304571 -0.432130 -2.739336 C 0.909919 1.627882 -2.179903 H 0.314265 -0.415480 -1.934549 C 3.654422 0.240470 -2.457680 H 4.653864 -0.898445 -0.896600 H 4.815139 0.822414 -0.715720 C 2.374378 -1.958738 -2.624988 H 2.005606 -0.184382 -3.762479 H 0.763787 1.696296 -3.260201 H 1.720390 2.301503 -1.898683 H -0.003147 1.988884 -1.708507 H 4.417258 -0.157938 -3.131253 H 3.576535 1.308037 -2.676145 H 1.413304 -2.411139 -2.884238 H 2.631349 -2.282533 -1.613085 H 3.130176 -2.359432 -3.305590 H 0.775109 2.204076 1.394249 H 0.246913 -0.409528 2.855486 H 0.135437 -1.165883 0.446873	N 0.623479 3.328878 0.728121 C -0.104396 2.407634 0.165888 N 0.325386 1.184695 -0.257812 C 1.660650 0.931298 -0.103622 C 2.492491 1.866131 0.519343 C 1.948561 3.095612 0.944447 N 2.465394 -0.118376 -0.452528 C 3.737055 0.228585 -0.013117 N 3.784544 1.398797 0.568394 C 3.759265 -3.102847 -1.254377 C 2.180186 -1.375436 -1.215716 C 1.659453 -2.517773 -0.320432 C 2.441426 -3.734585 -0.832024 O 3.382673 -1.807557 -1.795161 H 4.571625 -0.430102 -0.180366 H 4.283129 -3.634704 -2.046072 H 4.434660 -2.958671 -0.405035 H 1.497556 -1.098344 -2.019098 H 0.581367 -2.648063 -0.401190 H 1.907374 -2.308011 0.721565 H 2.567637 -4.498704 -0.065441 H 1.940923 -4.181257 -1.693401 N 2.668279 4.037841 1.537520 H 3.653126 3.901851 1.709283 H 2.233018 4.905286 1.814663 C -1.276396 0.811455 -2.062728 C -2.599565 0.858557 -2.250355 C -0.702423 0.237511 -0.809088 C -3.549702 0.366283 -1.219235 O -3.172360 1.341459 -3.369064 C -1.681358 -0.183348 0.261655 C -3.007667 -0.181261 0.028266 O -4.752456 0.436511 -1.464252 H -4.135222 1.252711 -3.243575 C -1.128346 -0.715204 1.566000 C -3.975717 -0.782424 1.009769 C -2.003676 -1.836229 2.105446 C -1.009397 0.392207 2.644432 H -0.123925 -1.109783 1.389515 C -3.316467 -1.820038 1.875935 H -4.812689 -1.216015 0.457363 H -4.419908 0.012965 1.624565 C -1.313924 -2.880329 2.934817 H -0.723975 -0.054905 3.598005 H -1.967073 0.899006 2.774411 H -0.253159 1.135762 2.394327 H -3.956540 -2.581924 2.309082 H -0.588868 -3.436908 2.331163 H -2.029437 -3.589990 3.353249 H -0.755359 -2.428331 3.761036 H -1.160269 2.593410 0.013852 H -0.583215 1.161068 -2.817640 H -0.153529 -0.667300 -1.070123	N 0.081784 2.923701 -1.374747 C -0.455897 1.773694 -1.079671 N 0.200240 0.671411 -0.621009 C 1.559024 0.787963 -0.511997 C 2.196910 1.998463 -0.792431 C 1.424953 3.093840 -1.230744 N 2.547064 -0.083365 -0.141732 C 3.728126 0.645624 -0.208928 N 3.552492 1.883485 -0.591110 C 4.410161 -2.611445 1.060504 C 2.505689 -1.530764 0.229044 C 2.303238 -1.759800 1.739266 C 3.284052 -2.899379 2.042939 O 3.739809 -2.100574 -0.123405 H 4.671821 0.180660 0.019556 H 4.974323 -3.488944 0.750702 H 5.100796 -1.852246 1.441461 H 1.731086 -1.985546 -0.385676 H 1.272332 -2.013880 1.983515 H 2.574491 -0.855003 2.286207 H 3.619644 -2.894282 3.079681 H 2.829526 -3.868157 1.826371 N 1.947648 4.279753 -1.513089 H 2.939309 4.440784 -1.421445 H 1.352344 5.030467 -1.830201 C -0.711447 -1.393511 -1.547379 C -1.896398 -1.771197 -2.038444 C -0.585062 -0.580221 -0.298822 C -3.173131 -1.396707 -1.382132 O -2.025310 -2.503047 -3.161020 C -1.876685 -0.223345 0.414563 C -3.108944 -0.613040 -0.142083 O -4.218916 -1.766164 -1.911043 H -2.982692 -2.629782 -3.295948 C -1.840220 0.485894 1.625689 C -4.303122 -0.269653 0.495666 C -3.055581 0.847489 2.245610 C -0.541977 0.899626 2.271616 C -4.269994 0.463369 1.667518 C -3.064897 1.642642 3.522938 H -0.618387 0.856204 3.357310 H -0.277341 1.928865 2.008219 H 0.292312 0.262679 1.989128 H -5.197246 0.743050 2.153288 H -2.615871 1.077372 4.345486 H -4.084401 1.900628 3.808811 H -2.491427 2.567709 3.420206 H -1.526403 1.659617 -1.184432 H 0.200320 -1.663329 -2.067168 H 0.034680 -1.118024 0.417284 H -5.241264 -0.582702 0.056864
E'-Q(H)$^-$-G$^+$R' (TS)	**Eq'-Q(H)$^-$-G$^+$R' (TS)**	**Eqn'-Q(H)$^-$-G$^+$R' (TS)**
C -1.676783 -0.066612 -1.951532 C -2.879589 -0.594191 -2.385893 C -3.759208 -1.168002 -1.319520 C -3.329325 -1.110323 0.075581 C -2.147890 -0.524679 0.455828 C -1.333885 0.146476 -0.547446 O -3.258493 -0.639779 -3.622678 O -4.851047 -1.712521 -1.621052 C -4.221871 -1.851207 1.050709 C -3.756334 -1.842579 2.514038	C -1.700072 -0.271714 -2.021220 C -2.912101 -0.801002 -2.431503 C -3.832236 -1.252003 -1.336628 C -3.394332 -1.124209 0.047126 C -2.207836 -0.538275 0.399079 C -1.362991 0.040284 -0.632849 O -3.275516 -0.936247 -3.664875 O -4.955708 -1.742873 -1.607777 C -4.277780 -1.737180 1.112414 C -3.494179 -2.183394 2.317538	C 1.482563 1.136741 1.739791 C 2.587664 0.940427 2.551958 C 3.404664 -0.264477 2.242383 C 3.086594 -1.058203 1.035325 C 1.991856 -0.765697 0.182221 C 1.176157 0.412649 0.511371 O 2.898529 1.683384 3.564002 O 4.350112 -0.604234 2.984602 C 3.939317 -2.129576 0.714426 C 3.710142 -2.906998 -0.399837

C -2.230163 -1.775699 2.641705	C -2.341134 -1.607413 2.661144	C 2.646870 -2.616666 -1.273274
C -1.715474 -0.520279 1.910126	C -1.851653 -0.411261 1.866115	C 1.807567 -1.528483 -1.006631
C -2.166532 0.775645 2.612139	C -2.474362 0.877544 2.459786	C 0.740275 -1.186270 -2.022205
C -1.544046 -3.048242 2.131815	C -1.514975 -2.018355 3.845453	C 2.450782 -3.473704 -2.499831
N 2.387413 2.306776 1.474961	N 2.239691 2.222123 1.533093	N -2.630589 2.981476 -0.176248
C 3.536845 1.603755 1.230347	C 3.413296 1.553634 1.305818	C -3.760103 2.206404 -0.234320
N 3.539955 0.472374 0.550795	N 3.465401 0.440077 0.599492	N -3.731574 0.895492 -0.069806
C 2.325446 0.091671 0.128508	C 2.272992 0.037372 0.135189	C -2.500797 0.402581 0.129778
C 1.103396 0.734796 0.308883	C 1.030769 0.642170 0.301493	C -1.296543 1.098771 0.176385
C 1.074597 1.951419 1.075150	C 0.949218 1.842645 1.087368	C -1.309598 2.528736 0.063049
N 2.069240 -1.052619 -0.610028	N 2.066925 -1.089456 -0.643750	N -2.195318 -0.929388 0.344468
C 0.748008 -1.082949 -0.873642	C 0.752850 -1.148677 -0.941474	C -0.856637 -1.022449 0.532415
N 0.130928 -0.035699 -0.339715	N 0.094144 -0.134211 -0.391801	N -0.281556 0.166609 0.411748
O 0.139042 2.655084 1.410471	O -0.014959 2.514963 1.405255	O -0.398027 3.334292 0.156488
N 4.690399 2.081160 1.737897	N 4.538340 2.047410 1.859673	N -4.931120 2.818583 -0.493695
C 5.282890 -1.504772 -1.451533	C 5.308848 -1.408959 -1.436945	C -5.378000 -1.815830 0.947240
C 3.041491 -2.060384 -1.092906	C 3.080377 -2.048247 -1.140398	C -3.124277 -2.079950 0.386097
C 3.862635 -2.694991 0.044669	C 3.901190 -2.694341 -0.009172	C -3.946515 -2.234929 -0.906434
C 5.286197 -2.720439 -0.531321	C 5.334985 -2.654798 -0.558363	C -5.351476 -2.563362 -0.381351
O 3.940656 -1.468113 -2.000602	O 3.976372 -1.396224 -2.010103	O -4.026292 -1.935957 1.459265
H -1.008339 0.372466 -2.687371	H -1.013397 0.087855 -2.783210	H 0.812547 1.951982 1.996204
H -1.663247 1.499303 -0.473680	H -1.654268 1.395775 -0.646822	H 1.518413 1.275780 -0.595990
H -4.296981 -2.884059 0.690733	H -4.816787 -2.579506 0.672787	H 4.778151 -2.327639 1.369476
H -5.242961 -1.462743 0.982719	H -5.065012 -1.028956 1.415909	H 4.364954 -3.742554 -0.624386
H -4.135401 -2.734282 3.023573	H -3.896201 -3.002003 2.909109	H -0.139156 -1.834836 -1.929940
H -4.191474 -0.986754 3.035971	H -0.766382 -0.337872 1.976157	H 1.123099 -1.324858 -3.034784
H -1.978386 -1.660504 3.702584	H -2.195939 0.984904 3.512263	H 0.410534 -0.154527 -1.942737
H -0.621364 -0.545306 1.950952	H -3.563859 0.824796 2.397681	H 1.428512 -3.856776 -2.567977
H -1.852534 0.765078 3.661357	H -2.122350 1.752431 1.917689	H 3.131804 -4.325972 -2.485694
H -3.253048 0.880785 2.582079	H -0.515701 -2.339430 3.529369	H 2.639987 -2.911856 -3.420765
H -1.725354 1.644393 2.128540	H -1.981377 -2.837053 4.397615	H -2.708251 3.985503 -0.286494
H -0.458662 -2.978829 2.253281	H -1.369278 -1.178711 4.534664	H -0.329167 -1.938970 0.727416
H -1.748606 -3.215030 1.071179	H 2.245132 3.062347 2.099223	H -5.769855 2.265439 -0.410579
H -1.890610 -3.926430 2.684611	H 0.288910 -1.905883 -1.549202	H -5.026751 3.820482 -0.443035
H 2.429544 3.157813 2.023282	H 5.411800 1.628358 1.580723	H -6.040161 -2.252695 1.693469
H 0.248056 -1.842952 -1.448505	H 4.570209 2.980650 2.238191	H -5.613360 -0.757797 0.810529
H 5.543533 1.631835 1.443515	H 6.011495 -1.433326 -2.268707	H -2.484629 -2.941459 0.580084
H 4.758928 3.023285 2.088447	H 5.452001 -0.498307 -0.851043	H -3.526511 -3.011828 -1.543586
H 5.968210 -1.579861 -2.294623	H 2.507564 -2.778487 -1.712145	H -3.951417 -1.297409 -1.460625
H 5.465906 -0.580058 -0.899842	H 3.544828 -3.701516 0.201944	H -6.138185 -2.233457 -1.060466
H 2.433785 -2.790375 -1.628081	H 3.819031 -2.099785 0.899242	H -5.463067 -3.637251 -0.215074
H 3.478254 -3.682438 0.295953	H 6.082341 -2.589861 0.232951	C 2.973781 2.046766 -1.944280
H 3.816630 -2.068580 0.934045	H 5.544098 -3.540655 -1.162282	O 3.932478 1.758888 -1.223373
H 6.050233 -2.653105 0.243699	C -1.138261 3.339339 -1.292799	O 1.723381 1.905175 -1.615326
H 5.455355 -3.632500 -1.108126	O -0.061379 2.939074 -1.751767	C 3.175303 2.604838 -3.343235
C -1.288159 3.474294 -1.111688	O -2.048355 2.578185 -0.773086	H 2.565699 3.499332 -3.486845
O -0.247174 3.134766 -1.686370	C -1.479428 4.820293 -1.279394	H 4.224472 2.838677 -3.519447
O -2.111086 2.661027 -0.528290	H -2.524096 4.981997 -1.550893	H 2.844456 1.862988 -4.075533
C -1.687543 4.938050 -1.019880	H -1.339997 5.200024 -0.262687	
H -1.453576 5.299335 -0.013828	H -0.827025 5.374874 -1.953310	
H -1.135564 5.536856 -1.743902		
H -2.761256 5.060474 -1.172569		
E'-Q(H)$^-$-A$^+$R' (TS)	**Eq'-Q(H)$^-$-A$^+$R' (TS)**	**Eqn'-Q(H)$^-$-A$^+$R' (TS)**
N -1.469373 -3.730246 -0.539629	N -1.697463 -3.663230 -0.429202	N 0.409632 3.492550 -1.097219
C -0.483538 -2.872413 -0.587713	C -0.645747 -2.888209 -0.483836	C -0.175484 2.318643 -1.098182
N -0.553072 -1.516060 -0.450344	N -0.615212 -1.524153 -0.439204	N 0.331339 1.151942 -0.619075
C -1.804889 -1.027728 -0.191409	C -1.837082 -0.927824 -0.277021	C 1.631570 1.213889 -0.205006
C -2.909767 -1.890486 -0.138886	C -3.007362 -1.697689 -0.222173	C 2.313006 2.432489 -0.157842
C -2.728183 -3.271524 -0.327992	C -2.925211 -3.098517 -0.310684	C 1.664668 3.602992 -0.598702
N -2.311998 0.222825 0.068799	N -2.252765 0.372402 -0.124291	N 2.521339 0.265722 0.243821
C -3.677511 0.049417 0.238995	C -3.633509 0.317986 -0.009224	C 3.687800 0.966675 0.527886
N -4.066858 -1.190482 0.124237	N -4.115100 -0.893796 -0.061999	N 3.597166 2.251076 0.311572
C -2.579204 3.638187 -0.332735	C -2.179882 3.769813 -0.736947	C 4.431279 -2.272238 -0.696075
C -1.672351 1.546290 0.191596	C -1.501465 1.637802 -0.054174	C 2.497162 -1.208700 0.077562
C -2.010984 2.267370 1.514503	C -1.803415 2.469855 1.209913	C 3.120534 -1.961738 1.265734
C -3.008693 3.358757 1.102383	C -2.672838 3.626607 0.698091	C 4.039611 -2.990242 0.589813
O -2.173872 2.356398 -0.857304	O -1.888648 2.423234 -1.168267	O 3.238259 -1.553275 -1.083424
H -4.318577 0.891449 0.441842	H -4.212951 1.219343 0.106267	H 4.570427 0.458813 0.880419
H -1.727952 4.325879 -0.368861	H -1.264876 4.368588 -0.786854	H 4.690377 -2.933736 -1.521483
H -3.374170 4.012975 -0.976213	H -2.917204 4.177140 -1.427576	H 5.254520 -1.566571 -0.534517
H -0.605125 1.396358 0.083031	H -0.451383 1.385304 -0.109384	H 1.465696 -1.482750 -0.086028

H -1.096406 2.722101 1.891389	H -0.855066 2.851181 1.588058	H 2.339550 -2.407370 1.876182
H -2.385912 1.583514 2.274565	H -2.271845 1.877113 1.994007	H 3.690502 -1.287455 1.905023
H -4.038833 2.996917 1.131586	H -3.734189 3.369200 0.716016	H 4.901533 -3.251741 1.204164
H -2.943855 4.242662 1.736768	H -2.536634 4.538938 1.278685	H 3.489072 -3.903839 0.355202
N -3.734164 -4.143974 -0.299758	N -3.995574 -3.889927 -0.274926	N 2.239721 4.804975 -0.561741
H -4.679462 -3.832479 -0.139444	H -4.920619 -3.499327 -0.185013	H 3.177187 4.915502 -0.208242
H -3.551450 -5.127356 -0.428587	H -3.883929 -4.890598 -0.332181	H 1.744819 5.610438 -0.912825
C 1.442725 -1.289034 -1.819728	C 1.480461 -1.536142 -1.693634	C -0.292719 -0.888691 -1.755694
C 2.813686 -1.225917 -1.986521	C 2.862907 -1.573188 -1.758835	C -1.227938 -1.639559 -2.450169
C 0.738494 -0.771758 -0.642801	C 0.733903 -0.887531 -0.611032	C -0.545855 -0.060908 -0.580230
C 3.584937 -0.755179 -0.793267	C 3.585156 -1.035166 -0.559416	C -2.649202 -1.399530 -2.071440
O 3.434682 -1.524293 -3.079736	O 3.538809 -2.012309 -2.766768	O -0.947277 -2.454627 -3.410556
C 1.514421 -0.574718 0.575718	C 1.445202 -0.624638 0.626555	C -1.948846 0.230161 -0.238096
C 2.881566 -0.494039 0.462605	C 2.813997 -0.588726 0.593930	C -2.949284 -0.469357 -0.961212
O 4.828724 -0.601762 -0.861276	O 4.838520 -0.981936 -0.540032	O -3.577542 -1.962130 -2.687021
C 0.822180 -0.447861 1.930295	C 0.702808 -0.399460 1.931276	C -2.327399 1.059735 0.857543
C 3.769275 -0.101876 1.623179	C 3.608598 -0.075716 1.769243	C -4.299529 -0.296633 -0.606066
C 1.666544 0.357559 2.944668	C 1.453207 0.518135 2.878201	C -3.682417 1.249053 1.150742
C 0.467645 -1.832296 2.518709	C 0.439963 -1.753744 2.639895	C -1.302320 1.745122 1.733997
H -0.119407 0.090726 1.795839	H -0.273113 0.049813 1.731868	C -4.659985 0.560720 0.409133
C 3.089561 -0.207066 2.986067	C 2.779812 0.627256 2.800151	H -5.046867 -0.850721 -1.159314
H 4.122870 0.924418 1.458144	H 4.391449 0.593681 1.395847	C -4.126119 2.164416 2.266331
H 4.671255 -0.717438 1.600898	H 4.165130 -0.901402 2.237699	H -0.365921 1.195933 1.774186
C 1.661090 1.859783 2.642644	H -0.063397 -1.595684 3.596240	H -1.667922 1.824313 2.757955
H 1.210848 0.211312 3.930228	H 1.387873 -2.262282 2.827768	H -1.087538 2.765373 1.396862
H 0.056650 -1.711857 3.524791	H -0.189527 -2.413480 2.041249	H -5.706932 0.701433 0.656703
H 1.351114 -2.469836 2.584428	H 0.332195 -3.337801 -0.590719	H -3.823135 1.784355 3.247706
H -0.276601 -2.362545 1.926272	H 0.914845 -1.817328 -2.578363	H -5.212675 2.262643 2.270870
H 3.678529 0.324715 3.740205	H 0.697056 0.335822 -1.272087	H -3.695704 3.164788 2.166651
H 3.057941 -1.255048 3.299130	O 0.821583 1.274498 -2.114608	H -1.181947 2.240643 -1.485531
H 0.679658 2.290004 2.853759	C 1.103809 2.470764 -1.704564	H 0.738258 -0.961656 -2.092482
H 1.889559 2.067070 1.595966	O 1.297525 2.784499 -0.523514	H -0.247491 -0.772315 0.659395
H 2.390121 2.381414 3.270480	C 1.150871 3.512595 -2.808026	O 0.002632 -1.212784 1.757096
H 0.519278 -3.235893 -0.766655	H 0.126048 3.735622 -3.118064	C -0.709285 -2.238764 2.134974
H 0.831312 -1.534683 -2.684410	H 1.619941 4.429887 -2.453955	O -1.462272 -2.879278 1.401670
H 0.529437 0.469239 -1.257456	H 1.684358 3.130530 -3.679981	C -0.535726 -2.585708 3.602018
O 0.423918 1.397722 -2.101521	H 3.308359 1.249549 3.518292	H -1.044857 -3.518082 3.841596
C 0.653139 2.616721 -1.725604	C 0.639511 1.217917 3.931444	H 0.524831 -2.666674 3.849504
O 1.019515 2.942614 -0.590580	H -0.084288 1.904193 3.482052	H -0.951708 -1.779384 4.212263
C 0.407566 3.657349 -2.802777	H 0.062604 0.505485 4.530631	
H -0.671334 3.751961 -2.951731	H 1.277496 1.790482 4.607568	
H 0.811907 4.624402 -2.506102		
H 0.846866 3.342901 -3.751233		
E'-Q(H)H$^+$-GR' (TS)	**Eq'-Q(H)H$^+$-GR' (TS)**	**Eqn'-Q(H)H$^+$-GR' (TS)**
C -1.683964 0.099035 -1.896302	C -1.713743 0.029853 -1.962090	C -1.486383 -1.171462 1.649045
C -2.871208 -0.425550 -2.251623	C -2.905555 -0.482299 -2.321628	C -2.614650 -0.946685 2.352002
C -3.753944 -1.053287 -1.271732	C -3.810738 -1.085662 -1.342915	C -3.466491 0.196553 2.076798
C -3.323318 -1.098010 0.112139	C -3.378523 -1.127213 0.037558	C -3.097429 1.066537 0.959352
C -2.136033 -0.532467 0.490436	C -2.191364 -0.571959 0.420020	C -1.965336 0.797216 0.151453
C -1.322307 0.213096 -0.482052	C -1.356040 0.153588 -0.545906	C -1.150654 -0.401372 0.460306
O -3.332359 -0.432813 -3.533668	O -3.356779 -0.490776 -3.606145	O -3.005237 -1.735308 3.395970
O -4.830889 -1.541396 -1.685827	O -4.898505 -1.545404 -1.757305	O -4.465209 0.381748 2.802752
C -4.200197 -1.901584 1.044408	C -4.240032 -1.877080 1.023504	C -3.921509 2.164670 0.673716
C -3.726169 -1.939947 2.502875	C -3.436114 -2.426888 2.170167	C -3.628487 2.994095 -0.386484
C -2.198075 -1.879657 2.618336	C -2.282675 -1.879386 2.554798	C -2.540795 2.720748 -1.232601
C -1.680283 -0.598720 1.933317	C -1.795295 -0.610853 1.878776	C -1.728565 1.602436 -0.993981
C -2.109216 0.677258 2.685553	C -2.377543 0.623565 2.613447	C -0.643085 1.282920 -1.996490
C -1.518469 -3.132690 2.053919	C -1.441458 -2.402033 3.682841	C -2.283417 3.629365 -2.407647
N 2.448988 2.264683 1.524053	N 2.324508 2.136920 1.646726	N 2.598722 -2.993030 -0.305984
C 3.586121 1.558504 1.231605	C 3.483247 1.476213 1.331538	C 3.742135 -2.234161 -0.338502
N 3.561766 0.444618 0.520977	N 3.498731 0.408073 0.553723	N 3.738265 -0.930214 -0.112048
C 2.336695 0.090686 0.113009	C 2.289325 0.050300 0.103367	C 2.519057 -0.424903 0.111285
C 1.129055 0.745956 0.331716	C 1.064520 0.662719 0.342032	C 1.305012 -1.101178 0.118450
C 1.125430 1.931700 1.145742	C 1.016519 1.793627 1.227835	C 1.291749 -2.526839 -0.033810
N 2.049397 -1.037903 -0.642391	N 2.039195 -1.035586 -0.724541	N 2.233052 0.900286 0.400944
C 0.726541 -1.048305 -0.878995	C 0.719769 -1.062396 -0.980932	C 0.899281 1.006818 0.590220
N 0.135562 0.000378 -0.312846	N 0.097269 -0.063215 -0.360601	N 0.307218 -0.167094 0.405540
O 0.198234 2.618196 1.533797	O 0.062486 2.425600 1.642731	O 0.362313 -3.311754 0.060832
N 4.755174 2.012015 1.716728	N 4.631826 1.926710 1.866173	N 4.899086 -2.852302 -0.626990
C 5.245009 -1.521863 -1.533167	C 5.256223 -1.383939 -1.601834	C 5.426086 1.677843 1.067124
C 3.001394 -2.053796 -1.158508	C 3.022631 -1.993707 -1.290007	C 3.185123 2.032326 0.509892

C 3.825410 -2.720749 -0.041996	C 3.850581 -2.707861 -0.206107	C 4.017670 2.236690 -0.769112
C 5.241952 -2.753882 -0.635134	C 5.274298 -2.668893 -0.781493	C 5.429283 2.493097 -0.221032
O 3.895409 -1.455545 -2.063667	O 3.911431 -1.317932 -2.144444	O 4.074076 1.811039 1.577704
H -1.032108 0.565194 -2.625065	H -1.053381 0.481542 -2.692719	H -0.827821 -1.986329 1.925372
H -1.614171 1.483995 -0.331470	H -1.624245 1.419741 -0.402296	H -1.458162 -1.198012 -0.611903
H -4.250713 -2.918154 0.637153	H -4.755944 -2.682561 0.495252	H -4.785220 2.340630 1.301968
H -5.226328 -1.526151 0.989823	H -5.041871 -1.223036 1.397418	H -4.254384 3.855176 -0.592193
H -4.101824 -2.847576 2.983933	H -3.827194 -3.300420 2.683667	H 0.238603 1.921006 -1.867081
H -4.158399 -1.100760 3.052633	H -0.706376 -0.566305 1.961978	H -1.007457 1.459081 -3.009738
H -1.937532 -1.804025 3.679712	H -2.078545 0.608118 3.664583	H -0.326424 0.245344 -1.949126
H -0.586871 -0.635705 1.953207	H -3.468559 0.603519 2.565907	H -1.247189 3.977492 -2.428144
H -1.772482 0.624435 3.725226	H -2.011024 1.544069 2.163368	H -2.936423 4.501876 -2.369787
H -3.195054 0.789597 2.681509	H -0.447672 -2.690959 3.322502	H -2.465082 3.116229 -3.357623
H -1.671018 1.560744 2.225589	H -1.902203 -3.270078 4.158172	H 2.660493 -3.994497 -0.446924
H -0.432967 -3.072582 2.175542	H -1.286091 -1.633221 4.447789	H 0.385092 1.921601 0.826520
H -1.724931 -3.258070 0.987674	H 2.357545 2.926497 2.281169	H 5.748935 -2.314902 -0.557732
H -1.867990 -4.030562 2.571185	H 0.229345 -1.786984 -1.607945	H 4.974849 -3.855552 -0.677247
H 2.510786 3.093061 2.104584	H 5.490895 1.505996 1.548327	H 6.094548 2.056797 1.838744
H 0.209281 -1.797854 -1.452809	H 4.687354 2.820528 2.327427	H 5.631291 0.621826 0.878033
H 5.597386 1.548739 1.413364	H 5.939382 -1.384675 -2.449846	H 2.559315 2.893504 0.745140
H 4.842203 2.929075 2.124372	H 5.430523 -0.503618 -0.979559	H 3.623766 3.061502 -1.360875
H 5.917054 -1.592015 -2.387134	H 2.420299 -2.683010 -1.882132	H 3.998024 1.333741 -1.377589
H 5.448543 -0.609661 -0.968374	H 3.478289 -3.716902 -0.036031	H 6.208783 2.173954 -0.913351
H 2.374306 -2.763219 -1.699014	H 3.797145 -2.156123 0.731075	H 5.573166 3.552910 0.000616
H 3.430270 -3.707511 0.194408	H 6.037166 -2.653784 -0.002682	C -2.977489 -1.937392 -1.920145
H 3.797896 -2.111364 0.859893	H 5.454879 -3.529993 -1.428675	O -3.863601 -1.680141 -1.098419
H 6.015171 -2.710484 0.132334	C -1.144241 3.430181 -1.015986	O -1.705464 -1.797798 -1.702925
H 5.392406 -3.657556 -1.229878	O -0.103587 2.995853 -1.535497	C -3.315045 -2.445174 -3.312787
C -1.235309 3.484809 -1.012868	O -2.040268 2.696990 -0.448197	H -2.730895 -3.338799 -3.542523
O -0.224847 3.072198 -1.603129	C -1.427648 4.924911 -0.988557	H -4.378343 -2.665823 -3.397865
O -2.065358 2.735822 -0.368262	H -2.485402 5.125253 -1.167401	H -3.046148 -1.681392 -4.047839
C -1.562924 4.970306 -0.987258	H -1.182849 5.306082 0.007717	H -3.819116 -1.316032 3.731292
H -1.281208 5.371960 -0.009056	H -0.817122 5.450978 -1.722258	
H -1.007360 5.504724 -1.757633	H -4.230134 -0.924342 -3.554874	
H -2.634221 5.135607 -1.114755		
H -4.195005 -0.887172 -3.477066		
E'-Q(H)H$^+$-AR' (TS)	**Eq'-Q(H)H$^+$-AR' (TS)**	**Eqn'-Q(H)H$^+$-AR' (TS)**
N -1.697769 -3.602845 0.255635	N 1.624831 3.693251 -0.399893	N 0.637835 3.322103 -1.330237
C -0.679989 -2.788716 0.215887	C 0.593634 2.897666 -0.448855	C -0.014935 2.190863 -1.257362
N -0.697549 -1.447526 -0.052596	N 0.598872 1.529320 -0.428769	N 0.404641 1.045166 -0.652959
C -1.947884 -0.908171 -0.228395	C 1.838798 0.956206 -0.295791	C 1.686087 1.076330 -0.174825
C -3.075548 -1.738573 -0.263682	C 2.988165 1.755997 -0.249952	C 2.425628 2.259113 -0.183448
C -2.936463 -3.118620 -0.023861	C 2.870051 3.156536 -0.313200	C 1.868230 3.416418 -0.765122
N -2.425224 0.366966 -0.409381	N 2.287760 -0.333431 -0.167275	N 2.497951 0.120926 0.389766
C -3.797071 0.230146 -0.579921	C 3.669336 -0.244736 -0.076049	C 3.678823 0.789407 0.698634
N -4.214907 -1.004556 -0.502255	N 4.117816 0.979770 -0.120616	N 3.666193 2.056420 0.381483
C -3.040663 3.692815 -0.314866	C 2.299600 -3.732842 -0.772014	C 4.261543 -1.971330 -0.953629
C -1.816115 1.697170 -0.108499	C 1.571001 -1.620485 -0.085110	C 2.396803 -1.365534 0.270205
C -2.182229 2.190048 1.304490	C 1.912724 -2.440038 1.176987	C 3.289953 -2.093613 1.279121
C -3.371472 3.126854 1.061135	C 2.809523 -3.570998 0.654932	C 4.565132 -2.454326 0.475725
O -2.360974 2.621455 -1.019947	O 1.963642 -2.395309 -1.201845	O 2.829941 -1.769608 -1.004109
H -4.413612 1.092414 -0.767844	H 4.273012 -1.132557 0.017127	H 4.505376 0.275915 1.160919
H -2.363349 4.548976 -0.245547	H 1.400833 -4.356599 -0.807240	H 4.505199 -2.696021 -1.728060
H -3.911902 3.969639 -0.907662	H 3.037649 -4.120236 -1.473043	H 4.766785 -1.028173 -1.183661
H -0.752238 1.599557 -0.281795	H 0.512682 -1.402183 -0.125888	H 1.355386 -1.620178 0.375557
H -1.337199 2.751976 1.704062	H 0.980065 -2.849245 1.564965	H 2.762260 -2.992726 1.593889
H -2.398123 1.369378 1.987022	H 2.371942 -1.832650 1.955319	H 3.481226 -1.503416 2.173464
H -4.314635 2.577431 1.043926	H 3.862680 -3.281462 0.656282	H 5.456604 -1.968950 0.874615
H -3.449201 3.904342 1.820687	H 2.709675 -4.485212 1.239761	H 4.737701 -3.529657 0.496559
N -3.962697 -3.961756 -0.042995	N 3.917018 3.973284 -0.282389	N 2.501866 4.584694 -0.799095
H -4.894626 -3.631846 -0.242955	H 4.854013 3.605835 -0.217024	H 3.420283 4.683399 -0.394512
H -3.815614 -4.939912 0.155773	H 3.778543 4.971915 -0.320610	H 2.070587 5.379279 -1.246834
C 1.303827 -1.652724 -1.402339	C -1.486566 1.483146 -1.683741	C -0.348176 -1.054974 -1.576244
C 2.647322 -1.713048 -1.441357	C -2.832129 1.455597 -1.663068	C -1.367361 -1.753965 -2.115457
C 0.641541 -0.855253 -0.366023	C -0.725113 0.863889 -0.590797	C -0.553963 -0.088291 -0.507234
C 3.466536 -1.128151 -0.383853	C -3.568250 0.943264 -0.508733	C -2.750274 -1.446129 -1.799105
O 3.342571 -2.299479 -2.454038	O -3.602155 1.867568 -2.705090	O -1.178434 -2.749306 -3.029005
C 1.432690 -0.458140 0.800704	C -1.444054 0.597326 0.660114	C -1.947011 0.329509 -0.208941
C 2.797850 -0.522167 0.749548	C -2.807699 0.529399 0.651961	C -3.004203 -0.365892 -0.845973
O 4.710870 -1.198637 -0.506674	O -4.816903 0.912305 -0.576465	O -3.649217 -2.101428 -2.365067
H 4.279045 -2.166900 -2.208931	C -0.683859 0.371640 1.951948	H -2.077853 -3.043624 -3.264061

C 0.729976 0.141546 2.004251 C 3.700348 0.086090 1.794551 C 1.610079 1.221684 2.670609 C 0.294473 -0.941316 3.012477 H -0.178593 0.631039 1.654524 C 2.968976 0.611165 3.033424 H 4.254075 0.898698 1.308878 H 4.462125 -0.643332 2.082781 C 1.762938 2.458962 1.776934 H 1.108001 1.524995 3.595551 H -0.124924 -0.467793 3.904083 H 1.136662 -1.564137 3.317836 H -0.470771 -1.598202 2.598131 H 3.590379 1.356339 3.538191 H 2.820724 -0.202593 3.747896 H 0.799664 2.949179 1.615441 H 2.171649 2.202394 0.796826 H 2.429108 3.189599 2.244685 H 0.310465 -3.188601 0.389457 H 0.699727 -2.065931 -2.202150 H 0.539663 0.246205 -1.111602 O 0.457618 1.217278 -1.988085 C 1.547228 1.886993 -2.215653 O 2.640050 1.660229 -1.689218 C 1.370129 3.026713 -3.207109 H 0.914905 2.657225 -4.128705 H 0.689719 3.770490 -2.783523 H 2.325929 3.498781 -3.430901	C -3.590393 0.041130 1.841001 C -1.415555 -0.561193 2.900737 C -0.431991 1.726165 2.664627 H 0.293399 -0.064562 1.733456 C -2.742895 -0.671115 2.850742 H -4.390252 -0.616160 1.484086 H -4.116512 0.883673 2.312826 H 0.078353 1.561629 3.615305 H -1.383118 2.223475 2.863606 H 0.188921 2.396425 2.069484 H -0.394094 3.333391 -0.520472 H -0.949133 1.809924 -2.566226 H -0.650955 -0.297012 -1.197412 O -0.800059 -1.299839 -2.082632 C -1.077493 -2.487552 -1.658720 O -1.222718 -2.792473 -0.465291 C -1.182623 -3.542586 -2.747001 H -0.172948 -3.789642 -3.087722 H -1.656566 -4.446773 -2.366386 H -1.737064 -3.160913 -3.605959 H -3.258418 -1.300701 3.570337 C -0.575486 -1.274970 3.922210 H 0.127991 -1.962063 3.443115 H 0.024568 -0.571818 4.508979 H -1.196969 -1.848983 4.611678 H -4.519207 1.710454 -2.408535	C -2.257386 1.294142 0.786956 C -4.337513 -0.043203 -0.551565 C -3.596297 1.632002 1.027755 C -1.186049 1.961067 1.619243 C -4.625844 0.959037 0.347157 H -5.124474 -0.596578 -1.047609 C -3.964230 2.696593 2.030663 H -0.305150 1.334798 1.729873 H -1.558431 2.161619 2.623565 H -0.876571 2.924481 1.200578 H -5.656616 1.223008 0.555137 H -3.719440 2.386942 3.051889 H -5.034100 2.904305 1.993840 H -3.427940 3.630479 1.843144 H -1.007059 2.135134 -1.683980 H 0.666462 -1.249477 -1.905982 H -0.325732 -0.701307 0.718057 O -0.153582 -1.140840 1.882518 C -0.876222 -2.194590 2.143504 O -1.600154 -2.761575 1.323418 C -0.748960 -2.682680 3.574482 H 0.298294 -2.900244 3.797667 H -1.071849 -1.896000 4.260864 H -1.351442 -3.575824 3.733105
E'-Q^{2-}-G^{+}R'	**Eq'-Q^{2-}-G^{+}R'**	**Eqn'-Q^{2-}-G^{+}R'**
C 0.707437 0.702887 2.211730 C 1.477479 1.317426 1.024883 H 0.346390 1.482496 2.888696 H 1.368843 0.040814 2.778079 H -0.157936 0.119716 1.897432 C 2.068503 0.227758 0.122937 C 2.517950 2.325276 1.575708 H 0.763291 1.910344 0.441016 C 3.729023 2.451701 0.657169 C 3.462681 0.051451 -0.033734 H 2.889104 1.924574 2.529497 C 1.255578 -0.705893 -0.523017 C 1.870587 3.685419 1.851780 C 4.412558 1.098097 0.501008 H 3.407314 2.820845 -0.326033 C 1.767618 -1.793604 -1.247583 H 4.425252 3.193406 1.065109 C 4.044463 -1.047508 -0.740771 N -0.181383 -0.551857 -0.517575 H 1.543709 4.149018 0.914614 H 2.579398 4.365714 2.333167 H 0.996545 3.599374 2.503009 C 3.147259 -2.038234 -1.369828 H 4.836392 0.798340 1.472703 H 5.266770 1.162241 -0.178040 H 1.074258 -2.476894 -1.730091 O 5.330264 -1.171884 -0.841475 C -0.820530 0.477395 -1.070071 C -1.146450 -1.407413 0.021702 O 3.617264 -3.062241 -2.022382 N -2.153140 0.352054 -0.886014 H -0.350565 1.280608 -1.605780 C -1.066590 -2.598883 0.811814 C -2.388541 -0.831610 -0.217489 N -3.598552 -1.288377 0.137761 O -0.091162 -3.216701 1.209937 N -2.371552 -3.041306 1.144196 C -3.552770 -2.422468 0.817334 H -2.392101 -3.891402 1.695216 N -4.697928 -3.019585 1.193705 H -4.707163 -3.801036 1.829139	C 1.065708 0.528061 2.426189 C 1.395632 1.271406 1.107907 H 0.608213 1.199227 3.158795 H 1.980225 0.115633 2.859840 H 0.372426 -0.296384 2.246211 C 2.046143 0.332145 0.106188 C 2.254459 2.482954 1.404259 H 0.445165 1.638799 0.707372 C 3.582324 2.415528 1.286090 C 3.450233 0.228632 0.024952 C 1.303554 -0.543815 -0.678627 C 1.533281 3.716589 1.873705 C 4.312007 1.194085 0.805865 C 1.897808 -1.500196 -1.515859 H 4.185139 3.282895 1.548702 C 4.118242 -0.734994 -0.787790 N -0.141634 -0.500733 -0.630362 H 0.841407 4.078285 1.103648 H 2.230282 4.522365 2.114530 H 0.928000 3.512473 2.763978 C 3.295495 -1.647259 -1.613734 H 4.780969 0.687912 1.666748 H 5.162738 1.490540 0.182328 H 1.262678 -2.151475 -2.109949 O 5.411594 -0.810839 -0.814730 C -0.875928 0.469743 -1.169408 C -1.014519 -1.397682 -0.011650 O 3.845414 -2.529210 -2.395515 N -2.184501 0.262916 -0.909059 H -0.485727 1.294883 -1.736135 C -0.810535 -2.580853 0.768240 C -2.302926 -0.912222 -0.193043 N -3.457066 -1.439263 0.241606 O 0.226222 -3.139528 1.092505 N -2.060915 -3.097451 1.188578 C -3.296608 -2.554773 0.934662 H -1.995156 -3.946738 1.737413 N -4.375664 -3.211562 1.397480 H -4.294162 -3.969587 2.055834 H -5.271061 -2.756643 1.312544 C -3.307861 1.159249 -1.306523 C -3.979886 1.804589 -0.075947	C 0.334360 1.411197 1.677363 C 1.743433 1.345482 1.127305 H 0.321703 1.916101 2.642079 H -0.088938 0.419458 1.833610 H -0.353145 1.964429 1.027164 C 2.150800 0.315711 0.198334 C 2.667197 2.275604 1.584799 C 4.030320 2.169512 1.199453 C 3.561450 0.167499 -0.107354 C 1.313387 -0.631197 -0.429964 C 2.279182 3.401498 2.518988 C 4.458786 1.132407 0.411664 C 1.817248 -1.672027 -1.217235 H 4.738533 2.905922 1.566440 C 4.111550 -0.905661 -0.918121 N -0.123741 -0.505594 -0.425733 H 1.420974 3.970104 2.149801 H 3.112364 4.096951 2.637362 H 2.014763 3.037560 3.518365 C 3.186183 -1.894526 -1.473320 H 5.506036 1.022313 0.157775 H 1.105223 -2.347429 -1.684321 O 5.373714 -0.981792 -1.143601 C -0.786383 0.483704 -1.023761 C -1.067458 -1.373247 0.128216 O 3.601414 -2.890780 -2.198675 N -2.117452 0.318796 -0.855102 H -0.331309 1.286579 -1.573274 C -0.956425 -2.535420 0.955469 C -2.323627 -0.846347 -0.144901 N -3.521515 -1.328622 0.216599 O 0.037044 -3.111086 1.373572 N -2.249230 -3.004806 1.297226 C -3.446000 -2.433681 0.940607 H -2.248830 -3.836083 1.876655 N -4.575796 -3.049376 1.333740 H -4.565779 -3.796863 2.009026 H -5.447851 -2.568726 1.177315 C -3.183877 1.240039 -1.333915 C -3.868091 1.981497 -0.168345 H -3.870802 0.624976 -1.915055 C -3.908300 3.434134 -0.665453

H -5.557888 -2.512022 1.057259 C -3.190835 1.333155 -1.309745 C -3.851981 2.018658 -0.095197 H -3.893192 0.779844 -1.932169 C -3.772976 3.510921 -0.455112 H -3.275636 1.804450 0.806017 H -4.868472 1.661283 0.056661 C -2.524068 3.563045 -1.323045 H -4.646223 3.818015 -1.034233 H -3.697555 4.148289 0.425933 H -2.505201 4.375360 -2.046892 H -1.609382 3.591207 -0.721595 O -2.568421 2.325009 -2.081838	H -3.985104 0.548957 -1.902976 C -4.012764 3.297043 -0.442761 H -3.366994 1.634679 0.810326 H -4.965231 1.379926 0.104884 C -2.798419 3.428212 -1.350092 H -4.922472 3.541823 -0.994820 H -3.952664 3.942387 0.433606 H -2.855360 4.237229 -2.075537 H -1.868858 3.517379 -0.777877 O -2.786808 2.187004 -2.105124	H -3.257213 1.895654 0.731801 H -4.850479 1.564870 0.044851 C -2.661621 3.504579 -1.535691 H -4.800338 3.613801 -1.269188 H -3.889451 4.155136 0.151845 H -2.706020 4.242273 -2.334620 H -1.757111 3.668099 -0.940849 O -2.593534 2.199602 -2.171136
E'-Q^{2-}-A^{+}R'	**Eq'-Q^{2-}-A^{+}R'**	**Eqn'-Q^{2-}-A^{+}R'**
N 2.585965 -2.600293 1.359531 C 1.362615 -2.145948 1.481991 N 0.866668 -1.009824 0.927566 C 1.759650 -0.274647 0.206478 C 3.065423 -0.710935 -0.005955 C 3.478200 -1.918377 0.594612 N 1.633222 0.918078 -0.455013 C 2.876327 1.140910 -1.036199 N 3.746625 0.193633 -0.795740 C 1.596738 3.829371 0.405179 C 0.530258 1.917494 -0.331154 C 0.478301 2.867033 -1.532774 C 1.264440 4.118834 -1.069857 O 0.743098 2.730692 0.795670 H 3.066803 2.018114 -1.632556 H 1.376568 4.655446 1.078952 H 2.644033 3.539180 0.538021 H -0.376196 1.345714 -0.169469 H -0.566940 3.113245 -1.713303 H 0.865425 2.413579 -2.443300 H 2.171439 4.277103 -1.654545 H 0.650800 5.013785 -1.166202 N 4.705062 -2.415931 0.449989 H 5.392594 -1.936331 -0.109974 H 4.955786 -3.278135 0.909341 C -0.943908 -0.025331 2.238688 C -2.261627 0.437660 2.427469 C -0.542741 -0.662209 1.055542 C -3.193765 0.247347 1.296516 O -2.639085 1.026432 3.523461 C -1.399351 -0.890480 -0.017813 C -2.727028 -0.424837 0.124011 O -4.409106 0.688065 1.371130 C -0.933102 -1.639396 -1.260626 C -3.722441 -0.557303 -1.008943 C -1.793204 -1.289493 -2.491842 C -0.895337 -3.162065 -1.022909 H 0.092589 -1.334837 -1.499382 C -3.276596 -1.475053 -2.151055 H -3.935616 0.445064 -1.406907 H -4.681531 -0.899550 -0.607629 C -1.495329 0.122551 -3.006689 H -1.528599 -1.996525 -3.287216 H -0.576977 -3.687783 -1.929170 H -1.877867 -3.541402 -0.733448 H -0.197964 -3.424062 -0.224936 H -3.889708 -1.288138 -3.039491 H -3.449506 -2.519435 -1.872974 H -0.440433 0.223256 -3.277912 H -1.719486 0.876693 -2.249362 H -2.094980 0.350958 -3.892905 H 0.644201 -2.704808 2.067569 H -0.211617 0.146971 3.022345	N -3.190773 -2.307408 -0.673305 C -1.899996 -2.185551 -0.867017 N -1.170084 -1.051072 -0.718781 C -1.876277 0.056228 -0.354479 C -3.249353 0.007165 -0.114942 C -3.914444 -1.224631 -0.283372 N -1.492003 1.347535 -0.137335 C -2.648976 2.020462 0.225908 N -3.712291 1.255373 0.248363 C 0.200163 4.297644 -0.082604 C -0.155950 1.982969 -0.262561 C 0.503336 2.263031 1.094034 C 1.188659 3.611817 0.853398 O -0.329727 3.233198 -0.911783 H -2.629635 3.076373 0.440703 H 0.648795 5.033798 -0.748568 H -0.619806 4.768240 0.471141 H 0.436489 1.324366 -0.892323 H 1.186175 1.464135 1.374230 H -0.263203 2.352596 1.867449 H 1.352545 4.173396 1.773479 H 2.150792 3.472327 0.354488 N -5.222284 -1.373831 -0.079891 H -5.791455 -0.592220 0.205445 H -5.654034 -2.274611 -0.219168 C 0.692981 -0.786261 -2.275424 C 2.055229 -0.616955 -2.600947 C 0.265857 -1.024668 -0.958120 C 3.017029 -0.667465 -1.474346 O 2.455346 -0.416460 -3.818604 C 1.140723 -1.084705 0.117878 C 2.509267 -0.893469 -0.160321 O 4.282846 -0.505050 -1.687606 C 0.659623 -1.381053 1.527243 C 3.501867 -0.878824 0.978490 C 1.586144 -0.818619 2.585790 C 0.488935 -2.903969 1.750210 H -0.326554 -0.924973 1.678689 C 2.880877 -0.630752 2.322699 H 4.257828 -0.113888 0.771647 H 4.078169 -1.819198 1.006955 C 0.971721 -0.525051 3.926083 H 0.167652 -3.123425 2.772247 H 1.438404 -3.413966 1.569833 H -0.255150 -3.321491 1.068461 H 3.535667 -0.267151 3.112171 H 0.202607 0.251213 3.834963 H 1.720230 -0.183189 4.644146 H 0.475541 -1.407693 4.344101 H -1.324684 -3.048458 -1.176481 H -0.046535 -0.717910 -3.068625	N -3.410243 -2.029977 -0.788225 C -2.111536 -2.041572 -0.960712 N -1.259236 -1.015774 -0.709482 C -1.841821 0.137404 -0.274574 C -3.213867 0.221061 -0.036616 C -4.011646 -0.909315 -0.307166 N -1.321318 1.361799 0.033854 C -2.401472 2.127090 0.448511 N -3.540915 1.481712 0.419302 C 0.622640 4.149888 0.162393 C 0.064477 1.882466 -0.096057 C 0.776207 2.050638 1.253097 C 1.567865 3.345753 1.047076 O -0.012806 3.167938 -0.693649 H -2.271317 3.157375 0.737262 H 1.118377 4.871513 -0.485848 H -0.142860 4.665696 0.752753 H 0.584499 1.205782 -0.767649 H 1.392570 1.186498 1.486489 H 0.036462 2.171079 2.048166 H 1.799195 3.854011 1.983516 H 2.503473 3.144594 0.519549 N -5.329510 -0.927215 -0.116462 H -5.809556 -0.114513 0.237626 H -5.857837 -1.759226 -0.330669 C 0.556053 -0.878019 -2.278252 C 1.888473 -0.691600 -2.705963 C 0.170986 -1.121736 -0.953448 C 2.897754 -0.645479 -1.645376 O 2.194193 -0.521281 -3.956328 C 1.099772 -1.180124 0.106902 C 2.468046 -0.897877 -0.279902 O 4.126499 -0.389066 -1.912398 C 0.804631 -1.465634 1.492233 C 3.446885 -0.837220 0.742327 C 1.802559 -1.366355 2.450854 C -0.574326 -1.914936 1.926565 C 3.128742 -1.036421 2.059881 H 4.463232 -0.613128 0.442654 C 1.541495 -1.607962 3.922327 H -1.305160 -1.100030 1.946658 H -0.548902 -2.333339 2.930131 H -0.965878 -2.693532 1.270351 H 3.896732 -0.962561 2.823304 H 0.728448 -0.984949 4.305968 H 2.435831 -1.379527 4.504959 H 1.273800 -2.649329 4.131182 H -1.631081 -2.940205 -1.325765 H -0.226068 -0.801050 -3.029151
E'-QH^{-}-G^{+}R'	**Eq'-QH^{-}-G^{+}R'**	**Eqn'-QH^{-}-G^{+}R'**
C 0.648101 0.712422 2.218334 C 1.405469 1.353598 1.037935	C 1.008041 0.466032 2.460587 C 1.317172 1.246870 1.160218	C 0.276051 1.403770 1.686024 C 1.700722 1.355878 1.176897

H 0.254530 1.484053 2.884754	H 0.510417 1.106809 3.192648	H 0.230599 1.904374 2.650833
H 1.328044 0.079689 2.795308	H 1.935266 0.092820 2.901756	H -0.139629 0.407986 1.830653
H -0.193221 0.097735 1.900555	H 0.357285 -0.387384 2.261419	H -0.395100 1.952313 1.017001
C 2.044156 0.280411 0.151145	C 2.014630 0.345534 0.155339	C 2.137122 0.371656 0.214825
C 2.397964 2.407513 1.596586	C 2.127035 2.486576 1.482192	C 2.614366 2.264251 1.700214
H 0.677277 1.906802 0.434978	H 0.359156 1.579454 0.750418	C 3.984822 2.184307 1.349849
C 3.643392 2.550937 0.726874	C 3.458559 2.466777 1.400053	C 3.549360 0.270359 -0.066835
C 3.441243 0.157149 0.039357	C 3.415962 0.311639 0.105222	C 1.301615 -0.543006 -0.484128
H 2.740750 2.044459 2.574852	C 1.294977 -0.516268 -0.677201	C 2.198339 3.346286 2.672136
C 1.250704 -0.648394 -0.538702	C 1.348048 3.689106 1.937163	C 4.439679 1.196943 0.515934
C 1.695584 3.751477 1.808204	C 4.236201 1.271402 0.929599	C 1.812802 -1.528364 -1.326349
C 4.356867 1.208317 0.613933	C 1.922017 -1.423307 -1.543231	H 4.677857 2.902642 1.774380
H 3.359800 2.904099 -0.273047	H 4.027292 3.349588 1.681561	C 4.097141 -0.750596 -0.933692
C 1.792246 -1.707217 -1.281149	C 4.100538 -0.596234 -0.745907	N -0.139258 -0.458653 -0.455665
H 4.308029 3.306697 1.158066	N -0.149320 -0.500567 -0.651147	H 1.353379 3.930980 2.299454
C 4.037185 -0.914549 -0.682553	H 0.667161 4.029918 1.148466	H 3.027616 4.032488 2.850471
N -0.188738 -0.533555 -0.538380	H 2.008138 4.517074 2.203432	H 1.901010 2.932519 3.641496
H 1.391879 4.178935 0.846683	H 0.725134 3.455474 2.807497	C 3.172734 -1.647797 -1.524825
H 2.361390 4.466845 2.299189	C 3.296168 -1.456916 -1.563935	H 5.491626 1.103347 0.276526
H 0.799600 3.650745 2.426507	H 4.678053 0.750353 1.793947	H 1.129631 -2.193140 -1.842989
C 3.157945 -1.839913 -1.330261	H 5.099019 1.593161 0.337083	O 5.346056 -0.888727 -1.200850
H 4.728882 0.910103 1.604752	H 1.334206 -2.077663 -2.176061	C -0.851915 0.477740 -1.080372
H 5.240261 1.279166 -0.025864	O 5.385404 -0.704855 -0.852328	C -1.033048 -1.335815 0.157529
H 1.142880 -2.400461 -1.802477	C -0.900161 0.454165 -1.198913	O 3.704668 -2.611229 -2.346653
O 5.309331 -1.111877 -0.817341	C -1.004266 -1.400517 -0.014402	N -2.166539 0.266787 -0.879566
C -0.866423 0.468484 -1.096724	O 4.002678 -2.302272 -2.378431	H -0.441005 1.280623 -1.664982
C -1.116920 -1.411518 0.025232	N -2.200179 0.228559 -0.933846	C -0.852016 -2.475097 1.005444
O 3.781262 -2.841525 -2.027802	H -0.524541 1.284369 -1.768966	C -2.313347 -0.876183 -0.113055
N -2.187807 0.299493 -0.899440	C -0.775290 -2.590356 0.748409	H 4.662677 -2.413689 -2.313034
H -0.429267 1.285087 -1.641127	C -2.299360 -0.938970 -0.197263	N -3.480060 -1.397896 0.285299
C -0.982856 -2.607844 0.801083	H 4.930234 -2.063164 -2.157661	O 0.178809 -2.996087 1.402023
C -2.378535 -0.882570 -0.207234	N -3.440521 -1.480087 0.248231	N -2.114013 -2.987256 1.389249
H 4.728813 -2.628381 -1.876682	O 0.275763 -3.139254 1.040267	C -3.342197 -2.476742 1.041814
N -3.565345 -1.375923 0.168557	N -2.012078 -3.120599 1.184450	H -2.066967 -3.803437 1.988435
O 0.023728 -3.197994 1.160430	C -3.257761 -2.590698 0.946223	N -4.435174 -3.119854 1.482061
N -2.264793 -3.087721 1.160564	H -1.931778 -3.974584 1.724293	H -4.385285 -3.872942 2.148835
C -3.471279 -2.504179 0.856104	N -4.321160 -3.251895 1.431776	H -5.333599 -2.698799 1.305435
H -2.250070 -3.941102 1.706994	H -4.225360 -4.018060 2.078587	C -3.281038 1.113030 -1.400442
N -4.588122 -3.124399 1.268171	H -5.226531 -2.818515 1.340702	C -4.053976 1.801304 -0.257519
H -4.566719 -3.928314 1.874228	C -3.339085 1.105695 -1.340852	H -3.898296 0.449996 -2.006247
H -5.470479 -2.661432 1.118173	C -4.025944 1.742336 -0.114422	C -4.148207 3.257565 -0.738440
C -3.262472 1.241887 -1.329332	H -4.001122 0.479597 -1.937830	H -3.480768 1.734112 0.668246
C -3.951252 1.902275 -0.116827	C -4.090276 3.231325 -0.490856	H -5.021937 1.332325 -0.094129
H -3.939814 0.659585 -1.952944	H -3.410531 1.591700 0.773603	C -2.878878 3.402064 -1.564941
C -3.935027 3.394693 -0.483974	H -5.001881 1.297366 0.067952	H -5.027487 3.402284 -1.369419
H -3.366174 1.717303 0.785226	C -2.874916 3.384589 -1.393112	H -4.191939 3.966288 0.088489
H -4.951401 1.502405 0.036989	H -5.002741 3.452225 -1.048274	H -2.932458 4.147275 -2.356046
C -2.685423 3.496437 -1.346060	H -4.048614 3.882755 0.381993	H -2.003134 3.599230 -0.938400
H -4.818066 3.660960 -1.068378	H -2.947424 4.186191 -2.125224	O -2.728564 2.110045 -2.215154
H -3.891206 4.038484 0.394445	H -1.950357 3.499516 -0.817684	
H -2.697385 4.304941 -2.074137	O -2.830270 2.137685 -2.139428	
H -1.775679 3.565059 -0.740694		
O -2.673451 2.253242 -2.099596		
E'-Q(H)H-A$^+$R'	**Eq'-Q(H)H-A$^+$R'**	**Eqn'-Q(H)H-A$^+$R'**
N 2.551781 -2.569239 1.467759	N -3.079132 -2.467122 -0.566301	N 3.301965 -2.271375 0.478159
C 1.334933 -2.097625 1.548507	C -1.794413 -2.304744 -0.744332	C 2.003833 -2.242993 0.626483
N 0.865125 -0.974220 0.939797	N -1.115679 -1.127110 -0.669459	N 1.209659 -1.140962 0.543171
C 1.781537 -0.277732 0.205699	C -1.876679 -0.025271 -0.402192	C 1.859632 0.038171 0.317400
C 3.086391 -0.735935 0.045014	C -3.249639 -0.122196 -0.179143	C 3.239537 0.083038 0.119321
C 3.471188 -1.925113 0.699738	C -3.857666 -1.391663 -0.266233	C 3.972583 -1.118549 0.206202
N 1.684969 0.888022 -0.505500	N -1.557694 1.295582 -0.280115	N 1.413355 1.324597 0.216793
C 2.947168 1.076564 -1.059272	C -2.752007 1.937272 0.016751	C 2.543861 2.086820 -0.043596
N 3.798672 0.130344 -0.758280	N -3.776693 1.125023 0.082382	N 3.644844 1.381320 -0.107115
C 1.624742 3.791808 0.352563	C -0.025910 4.329689 -0.454864	C -0.366414 4.208726 0.453144
C 0.586191 1.899678 -0.458461	C -0.256753 1.993274 -0.444799	C 0.053945 1.899282 0.403168
C 0.625974 2.849601 -1.659467	C 0.367626 2.418150 0.890961	C -0.624786 2.291283 -0.917643
C 1.400033 4.087503 -1.141570	C 0.981746 3.779010 0.547556	C -1.338658 3.595177 -0.546581
O 0.726453 2.706863 0.681015	O -0.486984 3.170874 -1.196460	O 0.187129 3.078589 1.175048
H 3.164039 1.929719 -1.680615	H -2.785759 3.005723 0.152867	H 2.475395 3.156625 -0.152609
H 1.372505 4.620328 1.011576	H 0.395197 5.027822 -1.176997	H -0.830936 4.863905 1.188690
H 2.654360 3.481371 0.556477	H -0.878471 4.801645 0.045012	H 0.443326 4.749572 -0.048671

H -0.337947 1.342989 -0.364090	H 0.380608 1.320209 -1.011090	H -0.512446 1.164703 0.967382
H -0.402157 3.112532 -1.903352	H 1.089817 1.685856 1.245750	H -1.291883 1.509461 -1.270961
H 1.061601 2.392785 -2.546252	H -0.414564 2.526062 1.645690	H 0.133525 2.466626 -1.683870
H 2.348106 4.229300 -1.661410	H 1.097419 4.421697 1.420427	H -1.515297 4.239137 -1.408276
H 0.809896 4.992643 -1.279304	H 1.958922 3.653680 0.075253	H -2.297016 3.385854 -0.065493
N 4.693168 -2.439326 0.605792	N -5.158467 -1.586105 -0.072862	N 5.290147 -1.175734 0.039985
H 5.400446 -1.987727 0.046548	H -5.768199 -0.813884 0.148079	H 5.821009 -0.341340 -0.157292
H 4.922720 -3.286618 1.103093	H -5.545831 -2.514329 -0.151370	H 5.770305 -2.059317 0.121371
C -0.930074 0.106049 2.185656	C 0.802158 -0.989022 -2.175312	C -0.627671 -1.217780 2.081671
C -2.235313 0.530332 2.264136	C 2.157702 -0.852590 -2.362860	C -1.960348 -1.089515 2.413904
C -0.535077 -0.600753 1.042428	C 0.322226 -1.071532 -0.858848	C -0.224305 -1.220667 0.745765
C -3.180967 0.296391 1.214237	C 3.082856 -0.775600 -1.267986	C -2.959953 -0.884219 1.428028
O -2.720302 1.233381 3.334317	O 2.726297 -0.766743 -3.603722	O -2.387433 -1.100712 3.717215
C -1.408337 -0.891033 -0.014090	C 1.165946 -1.015550 0.253771	C -1.147590 -1.091658 -0.330860
C -2.734056 -0.433368 0.074883	C 2.541852 -0.854079 0.044561	C -2.521856 -0.876274 0.047224
O -4.372894 0.769691 1.373812	O 4.333077 -0.635097 -1.556994	O -4.171955 -0.713544 1.807183
H -3.650821 1.395442 3.062250	H 3.678947 -0.666550 -3.382958	H -3.349642 -0.945795 3.630028
C -0.935419 -1.698857 -1.217279	C 0.621234 -1.167759 1.663876	C -0.819703 -1.134547 -1.735276
C -3.731524 -0.625045 -1.043338	C 3.484934 -0.712935 1.211794	C -3.484142 -0.629098 -0.953897
C -1.779543 -1.395647 -2.472389	C 1.491008 -0.480673 2.697924	C -1.798922 -0.854909 -2.682203
C -0.918888 -3.206303 -0.899386	C 0.464156 -2.664187 2.026558	C 0.562688 -1.512962 -2.220667
H 0.094550 -1.412222 -1.453751	H -0.375306 -0.716532 1.718864	C -3.130085 -0.590246 -2.276774
C -3.268336 -1.575199 -2.151117	C 2.797203 -0.313541 2.485006	H -4.506517 -0.459233 -0.640667
H -3.958345 0.361425 -1.468655	H 4.252084 0.024184 0.953233	C -1.498910 -0.827753 -4.164476
H -4.680316 -0.970972 -0.622147	H 4.045210 -1.648578 1.365794	H 1.293199 -0.707164 -2.101223
C -1.476445 -0.003443 -3.037238	C 0.803605 -0.047539 3.962102	H 0.545068 -1.760603 -3.278845
H -1.499654 -2.132042 -3.233962	H 0.091450 -2.781621 3.046768	H 0.944769 -2.391081 -1.700876
H -0.606850 -3.777392 -1.778557	H 1.429726 -3.169249 1.950707	H -3.875799 -0.374617 -3.034039
H -1.906325 -3.557392 -0.593207	H -0.235728 -3.165190 1.354765	H -0.664949 -0.161758 -4.400794
H -0.225172 -3.438860 -0.089694	H 3.411499 0.141752 3.257657	H -2.371501 -0.479832 -4.718993
H -3.867299 -1.411938 -3.052376	H 0.034413 0.702601 3.744904	H -1.239660 -1.819547 -4.548347
H -3.446446 -2.610304 -1.846149	H 1.510449 0.381813 4.674666	H 1.469625 -3.163276 0.825625
H -0.416569 0.092228 -3.289180	H 0.293814 -0.885810 4.448733	H 0.121297 -1.279855 2.863314
H -1.722426 0.783791 -2.320640	H -1.175887 -3.162420 -0.975603	
H -2.057202 0.182587 -3.945091	H 0.117603 -1.014111 -3.015008	
H 0.599023 -2.623068 2.143506		
H -0.216854 0.331593 2.969330		
E'-QH_2-G^+R'	**Eq'-QH_2-G^+R'**	**Eqn'-QH_2-G^+R'**
C -1.746285 -1.341284 1.554333	C 1.828818 -1.546962 -1.401499	C 1.763689 -1.672906 -1.081834
C -3.103153 -1.560545 1.711031	C 3.189991 -1.769777 -1.511009	C 3.110013 -1.997817 -1.271532
C -4.009516 -0.805791 0.956234	C 4.084545 -0.900394 -0.870342	C 4.080199 -1.096756 -0.882282
C -3.583218 0.149530 0.029848	C 3.632643 0.186516 -0.121518	C 3.738304 0.139377 -0.275644
C -2.204103 0.366706 -0.151292	C 2.252690 0.402820 0.020637	C 2.360683 0.456673 0.008813
C -1.328382 -0.386627 0.634335	C 1.388261 -0.471266 -0.637937	C 1.410472 -0.494881 -0.467731
O -3.543975 -2.489778 2.605787	O 3.648967 -2.821108 -2.246444	O 3.426616 -3.184994 -1.858643
O -5.324969 -1.074208 1.222645	O 5.403400 -1.209298 -1.062837	O 5.366049 -1.471193 -1.165474
C -4.633400 0.967140 -0.692500	C 4.623415 1.140922 0.503037	C 4.743885 1.079847 0.050364
C -4.082536 1.851050 -1.816648	C 4.024004 2.484959 0.811510	C 4.415672 2.263830 0.650619
C -2.731449 2.472276 -1.446166	C 2.715884 2.681948 0.973336	C 3.081211 2.568987 1.006630
C -1.697939 1.357529 -1.188172	C 1.748429 1.516973 0.915942	C 2.058231 1.671328 0.719392
C -1.293130 0.632664 -2.486004	C 1.481424 0.982315 2.343979	C 0.664672 2.000542 1.206422
C -2.836004 3.428260 -0.252287	C 2.119474 4.027881 1.271431	C 2.823701 3.883357 1.706184
N 2.084766 -2.591863 -1.477052	N -1.960033 -2.329698 1.873097	N -1.985529 -2.015603 2.198955
C 3.292410 -1.967539 -1.270567	C -3.181299 -1.771771 1.576092	C -3.204892 -1.533859 1.783680
N 3.414514 -0.865664 -0.544348	N -3.331289 -0.815632 0.670547	N -3.336730 -0.706019 0.756159
C 2.258128 -0.423250 -0.040652	C -2.188826 -0.448983 0.082013	C -2.180304 -0.397100 0.163567
C 1.001182 -0.985309 -0.194470	C -0.920091 -0.955048 0.314541	C -0.914815 -0.852408 0.496026
C 0.833322 -2.173740 -0.975488	C -0.722349 -1.986494 1.288032	C -0.732310 -1.721077 1.619577
N 2.087910 0.708164 0.751986	N -2.048255 0.527719 -0.899687	N -2.015921 0.459953 -0.921808
C 0.783429 0.805769 1.069027	C -0.750073 0.588217 -1.248438	C -0.707362 0.497623 -1.231877
N 0.098864 -0.188464 0.508011	N -0.040992 -0.281293 -0.531822	N -0.014594 -0.265371 -0.390078
O -0.187975 -2.792627 -1.228703	O 0.312861 -2.536294 1.629468	O 0.301989 -2.176667 2.080656
N 4.378435 -2.498666 -1.850665	N -4.251549 -2.212380 2.252869	N -4.294050 -1.909877 2.467999
C 5.362473 0.953178 1.429381	C -5.331688 0.600005 -1.565695	C -5.273064 0.400536 -1.700703
C 3.140926 1.645212 1.228036	C -3.122063 1.353990 -1.515100	C -3.076543 1.192190 -1.666594
C 3.929495 2.285753 0.071625	C -3.910193 2.168722 -0.473503	C -3.910404 2.110451 -0.754858
C 5.381349 2.210189 0.567229	C -5.365961 1.983870 -0.927360	C -5.347438 1.848484 -1.230122
O 4.048969 0.958244 2.049645	O -4.025677 0.524073 -2.197241	O -3.945243 0.274154 -2.276679
H -1.030365 -1.903645 2.138874	H 1.126331 -2.204739 -1.895803	H 1.000018 -2.358034 -1.426296
H -4.511220 -2.503628 2.582375	H 4.615824 -2.825576 -2.206831	H 4.391143 -3.258034 -1.896868
H -5.145410 1.593145 0.048885	H 5.474915 1.288158 -0.171907	H 5.780540 0.886309 -0.195744

H -5.398850 0.304724 -1.113386	H 5.044668 0.699331 1.418175	H 5.194649 2.983333 0.874006
H -4.808585 2.635614 -2.044228	H 4.715879 3.316288 0.903542	H 0.705632 2.744801 1.997360
H -3.971190 1.256385 -2.726271	H 0.798965 1.890467 0.523845	H 0.158518 1.132353 1.622929
H -2.376031 3.046872 -2.307719	H 1.120711 1.783623 2.992105	H 0.032643 2.416315 0.415969
H -0.799903 1.842931 -0.797210	H 2.401043 0.577936 2.772595	H 2.040208 4.461974 1.211183
H -0.953386 1.357741 -3.230214	H 0.732046 0.189924 2.335433	H 3.730773 4.488382 1.718917
H -2.129044 0.071129 -2.907398	H 1.422054 4.323447 0.479772	H 2.511475 3.735020 2.744630
H -0.480647 -0.072823 -2.310233	H 2.889605 4.796280 1.357760	H -1.940082 -2.624525 3.008293
H -1.873251 3.909304 -0.059240	H 1.546675 4.010111 2.204549	H -0.277406 1.062839 -2.041135
H -3.132153 2.906596 0.661872	H -1.902201 -3.050987 2.583029	H -5.193544 -1.608384 2.127505
H -3.573852 4.211745 -0.445315	H -0.339266 1.245857 -1.995808	H -4.266371 -2.618798 3.182987
H 2.048093 -3.427130 -2.050147	H -5.157167 -1.857463 1.988728	H -5.982761 0.147586 -2.486671
H 0.350362 1.575942 1.684807	H -4.211086 -3.010495 2.865998	H -5.366282 -0.301788 -0.869746
H 5.274607 -2.086828 -1.643127	H -6.070739 0.450233 -2.351085	H -2.536386 1.739497 -2.439302
H 4.359039 -3.391805 -2.315800	H -5.410109 -0.193389 -0.819453	H -3.599098 3.148365 -0.860449
H 6.092617 0.952751 2.237100	H -2.600590 1.981879 -2.237555	H -3.788268 1.817362 0.286822
H 5.466151 0.047227 0.828505	H -3.584934 3.207737 -0.466523	H -6.079753 1.989739 -0.434966
H 2.601510 2.377166 1.829055	H -3.759656 1.752475 0.521529	H -5.606472 2.505791 -2.062930
H 3.585749 3.301549 -0.116779	H -6.070180 2.041177 -0.097136	H 6.001707 -1.040626 -0.582533
H 3.801461 1.702530 -0.839179	H -5.639611 2.737630 -1.668797	
H 6.096910 2.141250 -0.252370	H 5.983048 -0.640558 -0.543666	
H 5.630057 3.083489 1.174125		
H -5.912084 -0.576855 0.641511		
E'-QH$_2$-A$^+$R'	**Eq'-QH$_2$-A$^+$R'**	**Eqn'-QH$_2$-A$^+$R'**
N -2.509545 -2.572848 -1.508093	N -2.959595 -2.612208 -0.447878	N -3.166875 -2.468513 -0.082086
C -1.305001 -2.076652 -1.567460	C -1.687926 -2.397760 -0.637047	C -1.875733 -2.390006 -0.238786
N -0.867993 -0.953688 -0.927547	N -1.070021 -1.180919 -0.623291	N -1.151526 -1.238498 -0.349991
C -1.805399 -0.288874 -0.187743	C -1.883611 -0.102113 -0.414103	C -1.870798 -0.076144 -0.331141
C -3.102983 -0.775206 -0.060228	C -3.249086 -0.260517 -0.183181	C -3.251932 -0.086447 -0.140956
C -3.454484 -1.960314 -0.742003	C -3.792464 -1.562191 -0.200661	C -3.910113 -1.327709 -0.013488
N -1.742710 0.862915 0.547566	N -1.635065 1.237946 -0.362329	N -1.506523 1.233393 -0.450440
C -3.019745 1.018977 1.079125	C -2.863387 1.829821 -0.096982	C -2.685984 1.956028 -0.320823
N -3.845951 0.062633 0.743748	N -3.841558 0.967897 0.013465	N -3.739301 1.202187 -0.137204
C -1.672637 3.744496 -0.359905	C -0.267858 4.338551 -0.732938	C 0.098380 4.132474 -1.235153
C -0.654902 1.888083 0.544882	C -0.377674 1.998774 -0.581649	C -0.187592 1.855224 -0.743714
C -0.769529 2.859201 1.722456	C 0.236662 2.533142 0.719166	C 0.450246 2.531348 0.478646
C -1.539678 4.070129 1.139335	C 0.775610 3.900945 0.288210	C 1.092150 3.779598 -0.135378
O -0.737590 2.668861 -0.615526	O -0.680126 3.113613 -1.395335	O -0.388701 2.854042 -1.722140
H -3.265196 1.858472 1.708233	H -2.955218 2.900504 -0.018965	H -2.685310 3.031098 -0.392573
H -1.396022 4.564699 -1.019161	H 0.111983 5.008239 -1.503027	H 0.535853 4.654056 -2.085000
H -2.682457 3.410014 -0.616781	H -1.138265 4.798579 -0.253748	H -0.744685 4.715644 -0.850533
H 0.281012 1.344704 0.518594	H 0.291746 1.333023 -1.119217	H 0.432744 1.068066 -1.161876
H 0.241950 3.145879 2.006446	H 1.001113 1.864183 1.108918	H 1.158374 1.874333 0.977578
H -1.236346 2.413245 2.598779	H -0.542731 2.644074 1.475984	H -0.326584 2.803536 1.196411
H -2.518607 4.197883 1.602123	H 0.864472 4.598943 1.120613	H 1.220272 4.585344 0.587374
H -0.978416 4.990511 1.294707	H 1.754032 3.798274 -0.186583	H 2.066837 3.538987 -0.565946
N -4.664606 -2.499618 -0.677731	N -5.078655 -1.812298 0.007490	N -5.219614 -1.437011 0.165565
H -5.390336 -2.072612 -0.122169	H -5.726798 -1.061465 0.191222	H -5.802426 -0.615366 0.220697
H -4.869057 -3.342502 -1.193818	H -5.418427 -2.762129 -0.021064	H -5.643549 -2.349482 0.244825
C 0.902912 0.171652 -2.140393	C 0.868033 -1.106695 -2.087906	C 0.707024 -1.562118 -1.803918
C 2.214374 0.604277 -2.239326	C 2.234870 -0.984519 -2.273823	C 2.065819 -1.513879 -2.131857
C 0.525437 -0.553626 -1.017415	C 0.367732 -1.080449 -0.789699	C 0.286938 -1.278959 -0.524761
C 3.109563 0.316542 -1.201884	C 3.069721 -0.814968 -1.159004	C 2.973788 -1.107734 -1.173763
O 2.611166 1.322197 -3.325924	O 2.752728 -1.013832 -3.531135	O 2.449688 -1.826480 -3.398549
C 1.400622 -0.881861 0.023504	C 1.176324 -0.939181 0.338741	C 1.181690 -0.940599 0.536075
C 2.725808 -0.421242 -0.077174	C 2.555677 -0.778785 0.138155	C 2.561127 -0.789916 0.147019
O 4.364278 0.827617 -1.382330	O 4.394100 -0.680961 -1.465120	O 4.264693 -1.008420 -1.607925
H 3.546446 1.548247 -3.222715	H 3.714695 -0.924346 -3.472069	H 3.412816 -1.747411 -3.456372
C 0.946233 -1.711372 1.215046	C 0.612100 -1.001428 1.744511	C 0.815167 -0.713505 1.908746
C 3.742553 -0.632059 1.024610	C 3.476271 -0.530252 1.309356	C 3.494460 -0.307992 1.094287
C 1.800556 -1.412472 2.464386	C 1.446333 -0.208878 2.730643	C 1.766833 -0.227122 2.799059
C 0.944423 -3.213302 0.870714	C 0.499802 -2.471954 2.215029	C -0.567601 -1.018843 2.438922
H -0.083757 -1.436491 1.460573	H -0.397427 -0.580166 1.747339	C 3.096972 -0.013317 2.369228
C 3.285686 -1.590667 2.129911	C 2.751323 -0.031143 2.527769	H 4.527955 -0.141370 0.817537
H 3.976474 0.346837 1.461288	H 4.235933 0.210085 1.031472	C 1.434479 0.088405 4.238241
H 4.680450 -1.008898 0.600669	H 4.032091 -1.447299 1.552979	H -0.553312 -1.074914 3.523710
C 1.499044 -0.026464 3.045222	C 0.726962 0.311525 3.941595	H -0.936174 -1.979211 2.083446
H 1.531563 -2.157149 3.220153	H 0.109677 -2.519371 3.233521	H -1.301614 -0.251990 2.176585
H 0.652931 -3.797932 1.746941	H 1.482483 -2.947685 2.197635	H 3.818636 0.378819 3.075935
H 1.930052 -3.548847 0.543316	H -0.169739 -3.046836 1.572764	H 1.198672 -0.816089 4.807117
H 0.239270 -3.441983 0.070343	H 3.347666 0.500335 3.262535	H 0.574554 0.757501 4.318736

H 3.895383 -1.425342 3.021572	H -0.055047 1.020750 3.648787	H 2.282745 0.570957 4.724239
H 3.466266 -2.621128 1.815929	H 1.410908 0.815323 4.626353	H -1.285975 -3.297189 -0.276862
H 0.441572 0.062665 3.307589	H 0.229377 -0.497352 4.486276	H -0.015071 -1.791639 -2.576888
H 1.735948 0.773740 2.339111	H -1.028079 -3.235287 -0.824503	H 4.894767 -1.040446 -0.879047
H 2.087428 0.149872 3.949410	H 0.208225 -1.208610 -2.939309	
H -0.552778 -2.573523 -2.166757	H 4.945495 -0.666804 -0.674477	
H 0.187175 0.417194 -2.913168		
H 4.954732 0.581815 -0.660542		
E'-QH_2-GH^{2+}R'	**Eq'-QH_2-GH^{2+}R'**	**Eqn'-QH_2-GH^{2+}R'**
C -1.844722 -1.370217 1.538468	C 1.960265 -1.430137 -1.492429	C 1.856640 -1.525457 -1.259695
C -3.220238 -1.497226 1.608364	C 3.339876 -1.526024 -1.525370	C 3.229519 -1.715945 -1.432560
C -4.024219 -0.689998 0.792459	C 4.111221 -0.643166 -0.754012	C 4.109602 -0.807150 -0.877541
C -3.477982 0.225969 -0.110745	C 3.518671 0.330779 0.050467	C 3.648276 0.296185 -0.113941
C -2.079183 0.351683 -0.204235	C 2.119131 0.418566 0.114338	C 2.241753 0.457644 0.159768
C -1.311590 -0.452123 0.641378	C 1.383183 -0.464894 -0.674353	C 1.391719 -0.481062 -0.495210
O -3.776902 -2.384678 2.477911	O 3.935172 -2.463567 -2.311986	O 3.660648 -2.774625 -2.170882
O -5.366527 -0.869196 0.975159	O 5.459377 -0.824059 -0.877123	O 5.426473 -1.038666 -1.155760
C -4.422903 1.102596 -0.905149	C 4.380464 1.302745 0.821187	C 4.560162 1.257427 0.382534
C -3.743873 1.927463 -2.003410	C 3.645840 2.555720 1.208832	C 4.115867 2.311121 1.132075
C -2.382231 2.467905 -1.553780	C 2.318170 2.627788 1.296449	C 2.752466 2.446840 1.483204
C -1.441910 1.294450 -1.213319	C 1.462886 1.398238 1.066515	C 1.819870 1.517369 1.035936
C -0.996313 0.526230 -2.471993	C 1.153945 0.709628 2.417992	C 0.398419 1.640062 1.536770
C -2.499611 3.449914 -0.382539	C 1.586159 3.884198 1.672417	C 2.362895 3.613416 2.359905
N 2.095249 -2.970710 -1.147516	N -1.929512 -2.899679 1.379553	N -2.012920 -2.750559 1.600107
C 3.326263 -2.455234 -0.922966	C -3.178007 -2.443309 1.124138	C -3.247638 -2.327855 1.241176
N 3.423957 -1.305312 -0.217624	N -3.316818 -1.374935 0.305730	N -3.347039 -1.306431 0.358545
C 2.279902 -0.710741 0.228273	C -2.194873 -0.796202 -0.211822	C -2.201734 -0.747405 -0.127152
C 1.026520 -1.215193 -0.000238	C -0.924800 -1.238553 0.049441	C -0.946080 -1.171491 0.219348
C 0.834211 -2.431305 -0.749637	C -0.689458 -2.370899 0.909403	C -0.751607 -2.235963 1.171667
N 2.154571 0.445276 0.952318	N -2.111616 0.289087 -1.044000	N -2.077985 0.299219 -1.003547
C 0.836652 0.634417 1.179992	C -0.802351 0.495512 -1.303376	C -0.757043 0.499386 -1.203721
N 0.133911 -0.342929 0.611670	N -0.064796 -0.403048 -0.653640	N -0.053012 -0.361682 -0.471969
O -0.194732 -2.986982 -1.046771	O 0.358322 -2.868994 1.241080	O 0.279102 -2.689956 1.603910
N 4.410057 -3.052037 -1.374410	N -4.235052 -3.019200 1.658854	N -4.332030 -2.886854 1.736685
C 4.716538 2.174322 -0.116226	C -4.693415 2.046832 -0.088916	C -4.682516 2.103899 -0.269786
C 3.293075 1.281678 1.501214	C -3.282547 1.040108 -1.649125	C -3.224412 0.998550 -1.711908
C 2.989534 2.786282 1.407381	C -3.017105 2.553566 -1.707797	C -2.964396 2.505216 -1.876554
C 4.253821 3.347094 0.732341	C -4.276234 3.147221 -1.050867	C -4.239013 3.139697 -1.289725
O 4.424194 1.012997 0.722384	O -4.391688 0.820301 -0.825411	O -4.365076 0.833717 -0.920118
H -1.206965 -1.969892 2.174081	H 1.351727 -2.096463 -2.089097	H 1.164894 -2.201937 -1.744342
H -4.740037 -2.330278 2.400585	H 4.894861 -2.385524 -2.214208	H 4.628499 -2.765167 -2.185027
H -4.932126 1.774445 -0.203194	H 5.251036 1.585612 0.217589	H 5.616366 1.187603 0.153683
H -5.206554 0.488831 -1.364193	H 4.788100 0.813376 1.717634	H 4.823480 3.052393 1.484066
H -4.400590 2.752561 -2.289920	H 4.254132 3.428528 1.423833	H 0.372676 2.212408 2.460705
H -3.613078 1.309408 -2.894668	H 0.512052 1.731987 0.643396	H -0.044800 0.673281 1.764448
H -1.934917 3.002219 -2.398068	H 0.689290 1.414692 3.109875	H -0.253412 2.162605 0.830365
H -0.544823 1.731907 -0.767328	H 2.075439 0.336442 2.869640	H 2.066025 3.284400 3.360801
H -0.553295 1.215648 -3.195037	H 0.472591 -0.132739 2.289131	H 1.525398 4.176024 1.941071
H -1.836725 0.017983 -2.948078	H 0.918382 4.197123 0.862067	H 3.204274 4.297267 2.474939
H -0.249233 -0.232117 -2.234745	H 2.277820 4.700991 1.885000	H -1.941691 -3.511211 2.269161
H -1.521774 3.872066 -0.135274	H 0.957676 3.728305 2.555446	H -0.329212 1.231697 -1.866789
H -2.885964 2.965323 0.518244	H -1.828507 -3.708786 1.984538	H -5.253902 -2.581055 1.458828
H -3.171421 4.275018 -0.633802	H -0.407164 1.263149 -1.946866	H -4.277980 -3.644081 2.402719
H 2.025957 -3.834795 -1.676244	H -5.170671 -2.695511 1.457100	H -5.750169 2.087061 -0.066137
H 0.412317 1.445652 1.746794	H -4.142779 -3.806907 2.283915	H -4.125570 2.174439 0.668552
H 5.328906 -2.668979 -1.202107	H -5.755667 2.014881 0.139873	H -3.357674 0.454549 -2.645199
H 4.356932 -3.909601 -1.904766	H -4.113115 2.058281 0.837459	H -2.794005 2.764057 -2.919353
H 5.784166 2.146498 -0.319138	H -3.457669 0.570539 -2.615135	H -2.092024 2.811261 -1.298694
H 4.157069 2.088990 -1.051652	H -2.863972 2.889034 -2.731334	H -4.040474 4.110658 -0.837745
H 3.459973 0.913000 2.511608	H -2.131819 2.807536 -1.123581	H -5.001259 3.260292 -2.060825
H 2.795955 3.213902 2.388934	H -4.066519 4.087360 -0.542243	H 6.011411 -0.604014 -0.524814
H 2.117755 2.959715 0.775026	H -5.057582 3.315957 -1.793348	H -4.235593 -0.879045 0.096104
H 4.039529 4.233465 0.136514	H 5.955885 -0.227034 -0.305677	
H 5.011839 3.597834 1.475936	H -4.214555 -0.932174 0.108365	
H -5.883606 -0.321606 0.372840		
H 4.307781 -0.822126 -0.056681		
E'-QH_2-AH^{2+}R'	**Eq'-QH_2-AH^{2+}R'**	**Eqn'-QH_2-AH^{2+}R'**
N 2.736330 -2.539079 1.134132	N -2.900049 -2.601886 -0.571335	N -3.099551 -2.475955 -0.371193
C 1.530489 -2.084596 1.307412	C -1.641486 -2.328787 -0.752836	C -1.817539 -2.333941 -0.531593
N 1.058190 -0.877894 0.874852	N -1.068922 -1.091800 -0.661068	N -1.132258 -1.153125 -0.490669

C 1.987108 -0.054885 0.310126	C -1.921738 -0.066569 -0.383943	C -1.890034 -0.035882 -0.312455
C 3.281729 -0.494708 0.072877	C -3.272074 -0.297747 -0.172158	C -3.261803 -0.125181 -0.126948
C 3.665187 -1.803837 0.468644	C -3.785465 -1.617533 -0.265248	C -3.894654 -1.396550 -0.145041
N 1.910660 1.267470 -0.080203	N -1.702697 1.290730 -0.272126	N -1.545479 1.300733 -0.292355
C 3.121860 1.615949 -0.547995	C -2.887469 1.867834 -0.002669	C -2.677969 2.001626 -0.104330
N 3.951167 0.584180 -0.478713	N -3.835078 0.942978 0.068288	N -3.710493 1.177932 0.004327
C 0.816009 4.215423 -1.233420	C -0.332733 4.391886 0.068611	C -0.019396 4.319041 -0.247080
C 0.803201 2.311295 0.117297	C -0.429425 2.107281 -0.438407	C -0.201050 1.997641 -0.491101
C -0.334155 2.163919 -0.899350	C 0.340715 2.264381 0.879335	C 0.519916 2.273219 0.838321
C -0.574665 3.612247 -1.347609	C 0.822566 3.717553 0.794236	C 1.055083 3.696006 0.630509
O 1.392439 3.557823 -0.063381	O -0.822326 3.377980 -0.862287	O -0.475052 3.223130 -1.097378
H 3.374618 2.601084 -0.897727	H -3.035567 2.926661 0.116166	H -2.733240 3.075217 -0.066763
H 0.835804 5.283151 -1.027970	H -0.049673 5.254734 -0.530370	H 0.335729 5.102309 -0.913030
H 1.434969 3.999024 -2.108669	H -1.142007 4.669553 0.749472	H -0.864404 4.694486 0.337200
H 0.502036 2.191987 1.154337	H 0.126337 1.601609 -1.223038	H 0.344698 1.355424 -1.175398
H -1.209506 1.701403 -0.452890	H 1.148361 1.543985 0.968242	H 1.301157 1.544829 1.031420
H -0.002523 1.551226 -1.735943	H -0.339435 2.132986 1.723018	H -0.192676 2.238337 1.664269
H -0.974392 3.668982 -2.359575	H 1.008281 4.150063 1.776780	H 1.187141 4.229324 1.571300
H -1.264895 4.116821 -0.669068	H 1.737697 3.785947 0.202749	H 2.010945 3.673197 0.103696
N 4.847843 -2.352062 0.264845	N -5.048099 -1.954398 -0.086194	N -5.183969 -1.610416 0.030100
H 5.600083 -1.897560 -0.230229	H -5.773698 -1.288453 0.132156	H -5.853261 -0.876661 0.207498
H 5.009237 -3.287837 0.613315	H -5.308971 -2.926843 -0.182513	H -5.524537 -2.561987 -0.010853
C -0.731802 0.168573 2.129523	C 0.781656 -0.727140 -2.192698	C 0.662046 -1.126064 -2.055740
C -2.062151 0.516741 2.281206	C 2.133802 -0.558630 -2.432711	C 2.003188 -0.998046 -2.424930
C -0.358247 -0.561357 1.005381	C 0.359990 -0.926407 -0.880155	C 0.302281 -1.119521 -0.726047
C -2.986841 0.114993 1.306766	C 3.033755 -0.579750 -1.353806	C 2.954603 -0.804053 -1.440063
O -2.454560 1.242402 3.360310	O 2.576268 -0.363464 -3.701786	O 2.330063 -1.030006 -3.743103
C -1.259004 -1.010163 0.031024	C 1.229972 -0.981011 0.206963	C 1.238780 -1.010681 0.344054
C -2.610678 -0.651657 0.199589	C 2.596754 -0.777854 -0.044229	C 2.601257 -0.777293 -0.065729
O -4.261887 0.537902 1.539298	O 4.334736 -0.382111 -1.709876	O 4.222880 -0.615660 -1.900410
H -3.409301 1.392102 3.304448	H 3.540212 -0.276022 -3.685769	H 3.289932 -0.935427 -3.826734
C -0.827290 -1.869256 -1.151363	C 0.759193 -1.279331 1.616662	C 0.932308 -1.080555 1.748364
C -3.677877 -1.002227 -0.815952	C 3.577771 -0.722678 1.103149	C 3.576369 -0.499864 0.921209
C -1.789059 -1.718299 -2.352025	C 1.626571 -0.591440 2.653633	C 1.922667 -0.785119 2.678139
C -0.712210 -3.355388 -0.750150	C 0.748435 -2.804996 1.876847	C -0.427008 -1.506303 2.256551
H 0.162116 -1.537976 -1.481633	H -0.266088 -0.920303 1.741248	C 3.234225 -0.477890 2.244491
C -3.226326 -1.991022 -1.895464	C 2.918547 -0.375259 2.410088	H 4.598567 -0.274899 0.643611
H -4.014971 -0.070964 -1.287611	H 4.350414 0.026040 0.895740	C 1.658636 -0.780754 4.165353
H -4.552739 -1.419582 -0.304497	H 4.108651 -1.681412 1.190446	H -0.384888 -1.722204 3.319780
C -1.659884 -0.368683 -3.062908	C 0.959212 -0.231202 3.948774	H -0.768496 -2.419823 1.770812
H -1.510028 -2.495462 -3.069999	H 0.448447 -3.011721 2.905875	H -1.196938 -0.741252 2.129465
H -0.526210 -3.964558 -1.637829	H 1.744103 -3.222695 1.715812	H 3.986842 -0.237219 2.985612
H -1.626004 -3.711450 -0.271987	H 0.050598 -3.321310 1.215203	H 0.810322 -0.143313 4.425020
H 0.108678 -3.537827 -0.058217	H 3.549981 0.072601 3.170382	H 2.532615 -0.411506 4.702154
H -3.909506 -1.928447 -2.745849	H 0.158143 0.496851 3.779674	H 1.440465 -1.785131 4.540310
H -3.301213 -3.010120 -1.510460	H 1.669297 0.195719 4.658635	H -1.201432 -3.206153 -0.709727
H -0.626699 -0.187108 -3.370963	H 0.494197 -1.107675 4.411914	H -0.092761 -1.201240 -2.827935
H -1.972949 0.463232 -2.430094	H -0.953800 -3.125427 -1.005591	H 4.885787 -0.761156 -1.215896
H -2.285809 -0.352815 -3.958996	H 0.074376 -0.697482 -3.010955	H -4.663893 1.491947 0.144244
H 0.805734 -2.685365 1.840213	H 4.933039 -0.480972 -0.960056	
H -0.004151 0.463103 2.874292	H -4.809690 1.149353 0.256816	
H -4.871702 0.225465 0.860445		
H 4.919699 0.627782 -0.772715		
E'-QH2-GH2+R' (TS)	**Eq'-QH2-GH2+R' (TS)**	**Eqn'-QH2-GH2+R' (TS)**
C -1.705008 -1.134344 1.763892	C 1.998397 1.116230 1.745052	C -1.527806 -1.168232 -1.807066
C -3.080417 -1.139357 1.914164	C 3.367045 1.142320 1.948515	C -2.860675 -1.526891 -2.036797
C -3.873081 -0.457220 0.983072	C 4.198535 0.351582 1.143250	C -3.814184 -1.209302 -1.092601
C -3.316556 0.209091 -0.111897	C 3.676082 -0.461459 0.137064	C -3.462405 -0.565465 0.122923
C -1.920030 0.198619 -0.286777	C 2.291898 -0.469076 -0.096783	C -2.081676 -0.286419 0.425859
C -1.154533 -0.468790 0.674092	C 1.485732 0.317583 0.727442	C -1.156512 -0.572961 -0.623898
O -3.647635 -1.785372 2.972729	O 3.892958 1.924218 2.933867	O -3.185426 -2.144919 -3.206980
O -5.214757 -0.489223 1.253978	O 5.530270 0.443343 1.446993	O -5.101226 -1.523786 -1.437527
C -4.241348 0.983190 -1.027973	C 4.593245 -1.351259 -0.669037	C -4.462600 -0.182139 1.046947
C -3.570900 1.518071 -2.298189	C 3.870792 -2.497517 -1.320899	C -4.121031 0.428269 2.222746
C -2.147030 2.016648 -2.028464	C 2.560927 -2.490837 -1.566939	C -2.769768 0.639906 2.580255
C -1.280026 0.857353 -1.498972	C 1.724030 -1.267143 -1.253318	C -1.749641 0.257230 1.714817
C -0.979417 -0.186960 -2.591196	C 1.603553 -0.378250 -2.515067	C -0.323024 0.385775 2.201111
C -2.118587 3.217610 -1.076034	C 1.841334 -3.642570 -2.208857	C -2.485293 1.270230 3.923368
N 2.025488 -3.477625 -0.746033	N -1.530831 3.058351 -1.402871	N 1.067907 3.418462 -0.952121
C 3.284060 -2.987004 -0.698841	C -2.805656 2.616166 -1.320131	C 2.412839 3.291745 -0.898382
N 3.468955 -1.732198 -0.242557	N -3.049551 1.483824 -0.632653	N 2.936508 2.059795 -0.739320

C 2.380136 -0.983956 0.152324	C -2.003644 0.798927 -0.050585	C 2.097073 0.970363 -0.636766
C 1.097775 -1.492117 0.095065	C -0.703453 1.254925 -0.149201	C 0.725445 1.111901 -0.696418
C 0.813312 -2.812740 -0.376545	C -0.358268 2.453588 -0.847760	C 0.087168 2.379435 -0.871199
N 2.387251 0.284431 0.629640	N -2.076616 -0.351650 0.658506	N 2.455954 -0.326543 -0.479328
C 1.101433 0.558035 0.870212	C -0.811385 -0.608161 1.000677	C 1.296527 -0.989388 -0.443637
N 0.283857 -0.470670 0.561638	N 0.056222 0.320957 0.539438	N 0.225579 -0.173169 -0.557993
O -0.249146 -3.383650 -0.495357	O 0.725470 2.971140 -1.017379	O -1.091172 2.653287 -0.944567
N 4.311604 -3.721537 -1.092008	N -3.790601 3.280997 -1.903229	N 3.195415 4.353451 -1.003616
C 2.849116 3.944898 0.073112	C -5.843367 -1.219433 1.605832	C 3.946480 -3.032015 1.773278
C 4.045366 2.051858 0.516882	C -3.774121 -2.163234 1.418205	C 4.599630 -1.388969 0.330484
C 3.850577 2.649224 1.851489	C -4.396649 -2.515959 0.133890	C 4.586081 -2.592833 -0.517587
C 2.794737 3.742901 1.588169	C -5.811987 -1.898708 0.231598	C 3.869901 -3.633453 0.369304
O 3.594307 2.743606 -0.440074	O -4.511765 -1.542514 2.225416	O 4.321011 -1.591356 1.543108
H -1.074887 -1.637848 2.485022	H 1.343586 1.714433 2.364741	H -0.793022 -1.342611 -2.582341
H -4.607436 -1.673819 2.921659	H 4.855452 1.824824 2.924200	H -4.136139 -2.326820 -3.201437
H -4.661850 1.819442 -0.455713	H 5.377975 -1.759578 -0.021118	H -5.510619 -0.340662 0.824174
H -5.091514 0.356167 -1.320628	H 5.119153 -0.757775 -1.431428	H -4.899695 0.740576 2.908850
H -4.180779 2.324596 -2.713037	H 4.472599 -3.358301 -1.595374	H 0.292468 -0.454563 1.889505
H -3.541426 0.729740 -3.053932	H 0.717889 -1.605372 -0.992962	H 0.157915 1.305813 1.857157
H -1.713421 2.333290 -2.982736	H 1.203041 -0.952606 -3.352963	H -2.032891 0.555523 4.618258
H -0.323085 1.289641 -1.196378	H 2.584938 0.008336 -2.798759	H -3.410256 1.628307 4.376547
H -0.538686 0.299449 -3.465438	H 0.940986 0.469912 -2.339580	H -1.800638 2.117447 3.838992
H -1.885256 -0.708423 -2.906251	H 1.071926 -4.038361 -1.536624	H 0.676056 4.346852 -1.066738
H -0.274796 -0.940158 -2.236804	H 2.528005 -4.452069 -2.462315	H 1.184438 -2.053951 -0.324363
H -1.097915 3.592352 -0.960024	H 1.327965 -3.329188 -3.123967	H 4.199888 4.276944 -0.943611
H -2.487876 2.955908 -0.080714	H -1.351458 3.913133 -1.918619	H 2.809945 5.280028 -1.110716
H -2.737450 4.033219 -1.459852	H -0.478164 -1.455482 1.578462	H 4.750032 -3.420967 2.393558
H 1.891371 -4.423444 -1.086977	H -4.743634 2.951121 -1.865740	H 3.012315 -2.999011 2.325222
H 0.719135 1.484537 1.264891	H -3.615090 4.124485 -2.428422	H 4.991619 -0.415217 0.072937
H 5.255332 -3.364922 -1.063467	H -6.572646 -1.616992 2.305333	H 5.641954 -2.841363 -0.696864
H 4.184693 -4.661882 -1.435687	H -5.882564 -0.133681 1.589304	H 4.136573 -2.405975 -1.491035
H 3.448404 4.791937 -0.251102	H -2.815941 -2.499932 1.789782	H 2.836167 -3.766616 0.055852
H 1.892146 3.931716 -0.439590	H -4.393918 -3.608927 0.052653	H 4.362648 -4.602208 0.331583
H 4.709956 1.239040 0.264613	H -3.785085 -2.144477 -0.690174	H -5.666947 -1.614103 -0.662360
H 4.828222 3.066233 2.131761	H -5.982030 -1.175848 -0.562743	H 3.940870 1.935273 -0.727296
H 3.591847 1.909718 2.606136	H -6.575529 -2.670201 0.165199	H -0.296914 0.406821 3.288045
H 1.806963 3.414080 1.905678	H 6.075277 -0.031666 0.809655	
H 3.028610 4.665041 2.115118	H -3.996781 1.141073 -0.541732	
H -5.724830 -0.043666 0.567668		
H 4.404813 -1.351685 -0.184684		
E'-QH2-AH2+R' (TS)	**Eq'-QH2-AH2+R' (TS)**	**Eqn'-QH2-AH2+R' (TS)**
N 2.913540 -2.466138 1.068420	N -3.032666 -2.564719 -0.437413	N -3.202234 -2.435313 -0.198258
C 1.675659 -2.105342 1.259178	C -1.755320 -2.381204 -0.622300	C -1.912360 -2.353976 -0.361067
N 1.123954 -0.922185 0.873416	N -1.119213 -1.178643 -0.611525	N -1.191878 -1.200302 -0.403465
C 1.980842 -0.012104 0.322990	C -1.906944 -0.082899 -0.409436	C -1.906815 -0.040746 -0.321933
C 3.308937 -0.351125 0.084980	C -3.274191 -0.221372 -0.196659	C -3.287957 -0.068758 -0.156315
C 3.784713 -1.636811 0.434661	C -3.860162 -1.509443 -0.209560	C -3.960152 -1.312374 -0.068927
N 1.757969 1.284898 -0.049853	N -1.560505 1.237496 -0.390233	N -1.472111 1.251773 -0.405738
C 2.929309 1.734888 -0.503577	C -2.695645 1.902886 -0.176765	C -2.566826 2.006873 -0.309175
N 3.876460 0.789248 -0.453541	N -3.740488 1.072429 -0.046002	N -3.669163 1.261028 -0.150496
C 0.453094 4.264464 -1.276963	C -0.173220 4.452642 -0.184971	C 0.178544 4.368288 -0.409537
C 0.420600 2.711791 0.417906	C 0.098061 2.288408 -0.913858	C 0.286731 2.114875 -0.863655
C -0.779976 2.410208 -0.410349	C 0.893924 2.379386 0.345264	C 0.974260 2.284830 0.452177
C -0.443619 3.118174 -1.731963	C 0.312071 3.637434 1.009227	C 0.468142 3.662106 0.910019
O 1.015712 3.798846 0.028553	O -0.383018 3.439620 -1.265940	O -0.051692 3.256769 -1.382207
H 3.111300 2.739923 -0.846400	H -2.786814 2.975018 -0.128958	H -2.590705 3.081848 -0.367660
H -0.086144 5.179685 -1.040460	H 0.573905 5.136475 -0.583003	H 1.029841 4.917599 -0.807319
H 1.300961 4.480547 -1.920494	H -1.120998 4.966981 -0.053216	H -0.711225 4.990958 -0.429510
H 0.515886 2.480255 1.469180	H 0.295875 1.594419 -1.718401	H 0.504683 1.329719 -1.573086
H -1.624481 2.886054 0.102905	H 1.932855 2.529771 0.026113	H 2.047552 2.297919 0.227208
H -0.993248 1.351556 -0.493165	H 0.868857 1.484041 0.954014	H 0.794279 1.475663 1.151238
H 0.093435 2.443368 -2.398410	H -0.513694 3.373132 1.670396	H -0.436302 3.557313 1.510126
H -1.331381 3.481649 -2.245336	H 1.056409 4.180175 1.587991	H 1.209988 4.199462 1.497158
N 5.008721 -2.087411 0.207895	N -5.145792 -1.767258 -0.026497	N -5.259740 -1.473803 0.121298
H 5.715087 -1.551551 -0.272139	H -5.836055 -1.051088 0.138330	H -5.902885 -0.707547 0.247698
H 5.245538 -3.021457 0.512869	H -5.456922 -2.728055 -0.064025	H -5.628019 -2.414328 0.159432
C -0.711741 -0.004519 2.162970	C 0.782982 -1.014383 -2.115831	C 0.598985 -1.291764 -1.966674
C -2.057485 0.284024 2.315213	C 2.146904 -0.895472 -2.325392	C 1.942121 -1.209549 -2.345137
C -0.300514 -0.676734 1.017317	C 0.314887 -1.074123 -0.805731	C 0.239578 -1.201603 -0.639907
C -2.957094 -0.104145 1.313145	C 3.010314 -0.812694 -1.221171	C 2.899335 -0.974000 -1.376020
O -2.487096 0.948175 3.420331	O 2.634504 -0.844682 -3.592750	O 2.265387 -1.331142 -3.659274

C -1.174686 -1.100319 0.009254 C -2.539859 -0.795161 0.171364 O -4.249743 0.265083 1.548071 C -0.688059 -1.864070 -1.214199 C -3.573008 -1.110772 -0.889854 C -1.618494 -1.642432 -2.426591 C -0.540754 -3.369353 -0.912217 H 0.299976 -1.481900 -1.488940 C -3.060622 -1.988043 -2.038347 H -3.943728 -0.159623 -1.291651 H -4.437093 -1.605443 -0.431653 C -1.499435 -0.232437 -3.011950 H -1.298289 -2.348708 -3.198779 H -1.468799 -3.789905 -0.521576 H 0.239398 -3.568670 -0.178397 H -0.274938 -3.907031 -1.825642 H -3.721478 -1.868579 -2.900253 H -3.116994 -3.038797 -1.746818 H -0.458734 0.005439 -3.247253 H -1.870546 0.530675 -2.325469 H -2.082294 -0.150920 -3.933015 H 0.998462 -2.779771 1.766051 H -0.001843 0.286684 2.926051 H -4.843229 -0.050153 0.856239 H -3.445823 1.066618 3.358414 H 4.836668 0.923239 -0.743668	C 1.150167 -1.018394 0.308707 C 2.526838 -0.857633 0.086755 O 4.326927 -0.669512 -1.550527 C 0.620279 -1.151965 1.722753 C 3.468913 -0.674597 1.253413 C 1.465433 -0.377099 2.715455 C 0.551575 -2.640691 2.139516 H -0.397318 -0.753707 1.765920 C 2.767876 -0.199410 2.496594 H 4.241936 0.057386 0.991923 H 4.004605 -1.612726 1.457982 C 0.759725 0.123113 3.942724 H 0.194372 -2.732313 3.167041 H 1.541521 -3.096550 2.074526 H -0.127151 -3.204370 1.496694 H 3.378136 0.316163 3.231043 H -0.016669 0.847039 3.670469 H 1.453186 0.604429 4.634013 H 0.256998 -0.693050 4.471764 H -1.116764 -3.235824 -0.805470 H 0.103397 -1.060652 -2.956776 H 4.899788 -0.728084 -0.777194 H 3.599100 -0.773993 -3.551978 H -4.692013 1.371900 0.123820	C 1.181556 -1.027942 0.417216 C 2.547702 -0.847858 -0.006771 O 4.171541 -0.839590 -1.847554 C 0.874831 -0.983048 1.823476 C 3.529765 -0.520190 0.957698 C 1.873450 -0.642934 2.729862 C -0.494848 -1.330496 2.362054 C 3.191026 -0.397433 2.275903 C 1.611668 -0.525373 4.212907 H -1.241947 -0.558396 2.162772 H -0.459557 -1.453404 3.440233 H -0.858367 -2.273485 1.955339 H 0.781233 0.151431 4.426746 H 2.496179 -0.142830 4.722369 H 1.367013 -1.494475 4.657755 H -1.330819 -3.261404 -0.464382 H -0.157429 -1.409396 -2.732137 H 4.831525 -0.978485 -1.158807 H 3.226735 -1.259234 -3.748966 H -4.604602 1.638249 -0.065260 H 4.554783 -0.332793 0.662909 H 3.949619 -0.119920 2.997862
E'-QH⁻-G	**Eq'-QH⁻-G**	**Eqn'-QH⁻-G**
C -0.470210 1.604562 -1.942918 C -0.956882 1.640812 -0.479823 H -0.071866 2.580804 -2.236296 H -1.287543 1.356086 -2.624552 H 0.313988 0.856409 -2.073764 C -1.409693 0.256707 -0.054694 C -2.049367 2.736868 -0.275107 H -0.094701 1.924473 0.127822 C -3.484796 2.171871 -0.229672 C -2.701767 -0.167173 -0.415727 H -1.984567 3.406606 -1.139928 C -0.559453 -0.632006 0.603916 C -1.762703 3.566545 0.980192 C -3.640822 0.855830 -1.000905 H -3.756208 1.975129 0.814559 C -0.959491 -1.945245 0.899746 H -4.184803 2.928450 -0.598378 C -3.146588 -1.485148 -0.146008 H -1.743268 2.921848 1.865628 H -2.533839 4.327142 1.137632 H -0.795762 4.073561 0.910925 N 0.759971 -0.215437 1.000215 C -2.219475 -2.351309 0.522368 H -3.447826 1.021883 -2.069319 H -4.664153 0.483061 -0.926616 H -0.284120 -2.620933 1.412296 O -4.315140 -1.976251 -0.433464 C 1.952268 -0.319147 0.294159 C 1.070226 0.441841 2.147249 H 0.308836 0.664538 2.879220 O -2.697055 -3.613736 0.775307 C 2.284840 -0.901419 -0.960954 C 2.922601 0.297862 1.090807 N 2.353699 0.767949 2.246184 H -3.604167 -3.556508 0.398479 N 4.239436 0.421814 0.764808 O 1.575175 -1.485663 -1.779044 N 3.663305 -0.730199 -1.217233 C 4.566486 -0.103902 -0.389375 H 3.986213 -1.138802 -2.085837 N 5.868885 -0.098257 -0.803566 H 6.470789 0.531744 -0.293791 H 6.061050 -0.156683 -1.792838	C -0.432661 1.880575 -1.520913 C -1.113814 1.714050 -0.140817 H -0.161660 2.924289 -1.700636 H -1.112190 1.560087 -2.314653 H 0.474057 1.277384 -1.583333 C -1.489466 0.261605 0.097120 C -2.309265 2.641234 -0.046976 H -0.387037 2.023450 0.615891 C -3.531965 2.202463 -0.352592 C -2.771101 -0.191821 -0.255421 C -0.563084 -0.651009 0.609746 C -2.022568 4.063171 0.348206 C -3.821577 0.778809 -0.734773 C -0.879025 -2.009006 0.766519 H -4.372256 2.892368 -0.330323 C -3.127704 -1.559306 -0.129622 H -1.598154 4.106511 1.357955 H -2.926697 4.675323 0.328917 H -1.285245 4.521819 -0.319827 N 0.753076 -0.216256 0.997212 C -2.131159 -2.442788 0.395351 H -3.941864 0.704192 -1.827735 H -4.792808 0.470662 -0.333582 H -0.144277 -2.697687 1.167852 O -4.279867 -2.073332 -0.436473 C 1.939488 -0.294499 0.277003 C 1.078635 0.380699 2.173179 H 0.327547 0.563628 2.926637 O -2.528181 -3.751713 0.514499 C 2.256272 -0.812262 -1.010193 C 2.919924 0.280051 1.092350 N 2.363685 0.698667 2.273665 H -3.452469 -3.706553 0.181779 N 4.234300 0.412782 0.760604 O 1.533631 -1.342923 -1.852910 N 3.634383 -0.641398 -1.268262 C 4.548680 -0.061126 -0.419404 H 3.946579 -1.007292 -2.159497 N 5.847716 -0.045470 -0.842935 H 6.458709 0.555853 -0.309939 H 6.033331 -0.063590 -1.834985	C 0.132065 2.186958 1.037368 C -1.176751 1.732060 0.428121 H 0.122635 3.257145 1.226239 H 0.987980 1.982252 0.389858 H 0.323722 1.695242 1.991297 C -1.500994 0.331083 0.280739 C -2.092090 2.702698 0.033254 C -3.360610 2.326270 -0.474290 C -2.815078 -0.017411 -0.209543 C -0.634663 -0.760496 0.577438 C -1.796277 4.184450 0.134905 C -3.714581 1.007217 -0.574987 C -1.050719 -2.082597 0.436501 H -4.058129 3.102180 -0.771571 C -3.256542 -1.387657 -0.350538 H -1.680182 4.511067 1.173169 H -2.614290 4.761233 -0.299689 H -0.879244 4.459201 -0.393408 N 0.740957 -0.600673 0.968459 C -2.327511 -2.389992 0.004859 H -4.690063 0.714768 -0.943174 H -0.349196 -2.880018 0.656185 O -4.420929 -1.744574 -0.775165 C 1.844699 -0.400367 0.149650 C 1.238118 -0.741381 2.224132 H 0.581884 -0.918722 3.062558 O -2.756334 -3.690792 -0.129730 C 1.980435 -0.189780 -1.250798 C 2.957068 -0.412966 0.996412 N 2.559294 -0.629810 2.291142 H -3.668767 -3.574767 -0.465232 N 4.245757 -0.228230 0.597246 O 1.124005 -0.139455 -2.132668 N 3.344230 -0.021980 -1.578760 C 4.395685 -0.041925 -0.691065 H 3.528148 0.107418 -2.566217 N 5.646728 0.089150 -1.223931 H 6.376027 0.269589 -0.549752 H 5.753256 0.575807 -2.101782

E'-QH^{--}-A	**Eq'-QH^{--}-A**	**Eqn'-QH^{--}-A**
N -3.092243 0.940929 -1.661573	N 2.991012 -1.072059 -1.649066	N 2.809210 0.141012 -1.929250
C -1.803030 1.048394 -1.435347	C 1.700086 -1.142062 -1.419196	C 1.554083 -0.105805 -1.634356
N -1.156982 0.674550 -0.305544	N 1.070097 -0.755413 -0.284199	N 1.070004 -0.413983 -0.408468
C -1.935839 0.145991 0.699274	C 1.867228 -0.248086 0.717488	C 1.989561 -0.505763 0.610007
C -3.325327 -0.010596 0.508134	C 3.259873 -0.133179 0.522372	C 3.354143 -0.254381 0.354945
C -3.896215 0.402462 -0.702284	C 3.814341 -0.562030 -0.690403	C 3.751532 0.080667 -0.945815
N -1.580545 -0.275927 1.920227	N 1.526415 0.192286 1.936129	N 1.797536 -0.781684 1.906754
C -2.779987 -0.683223 2.437700	C 2.738731 0.566458 2.449095	C 3.070003 -0.694110 2.404227
N -3.857257 -0.553958 1.653667	N 3.809952 0.400329 1.663824	N 4.042144 -0.384198 1.538193
H -2.843716 -1.089443 3.438800	H 2.816461 0.976817 3.447480	H 3.269491 -0.870172 3.453208
N -5.207250 0.295209 -0.973722	N 5.127488 -0.499151 -0.963526	N 5.022714 0.348720 -1.282947
H -5.842605 -0.065924 -0.281009	H 5.772703 -0.132250 -0.283085	H 5.752273 0.315472 -0.589665
H -5.571416 0.642351 -1.846577	H 5.475025 -0.826217 -1.850766	H 5.253023 0.587185 -2.234346
C 0.717820 2.171206 0.105639	C -0.866431 -2.192232 0.092871	C -0.684135 -2.036873 -0.278977
C 2.069937 2.382060 0.254353	C -2.227660 -2.350515 0.227061	C -2.002870 -2.439194 -0.188807
C 0.272780 0.870476 -0.167770	C -0.363445 -0.903989 -0.141330	C -0.340640 -0.688745 -0.222770
C 3.023536 1.321758 0.162036	C -3.141243 -1.251206 0.153579	C -3.061490 -1.509077 -0.073233
O 2.602815 3.617462 0.526720	O -2.811518 -3.571108 0.455968	O -2.363948 -3.765130 -0.240949
C 1.151036 -0.211377 -0.292419	C -1.200272 0.210311 -0.230526	C -1.318844 0.332735 -0.063890
C 2.529384 0.018476 -0.122477	C -2.583167 0.035377 -0.070416	C -2.693594 -0.111558 -0.022290
O 4.271264 1.626690 0.351996	O -4.402886 -1.512213 0.305270	O -4.270613 -1.951571 -0.028353
H 3.561434 3.406205 0.588374	H -3.762495 -3.327168 0.509269	H -3.340117 -3.717944 -0.181720
C 0.622631 -1.596954 -0.643959	C -0.641455 1.583146 -0.560549	C -1.054123 1.748692 0.061540
C 3.543768 -1.100909 -0.164458	C -3.512691 1.222604 -0.094613	C -3.729179 0.843833 0.063736
C 1.581139 -2.709623 -0.172048	C -1.504141 2.703658 -0.015537	C -2.112055 2.649283 0.123075
C 0.327005 -1.711632 -2.151858	C -0.474656 1.747357 -2.090578	C 0.355961 2.288506 0.173203
H -0.324069 -1.745389 -0.116953	H 0.350635 1.679755 -0.111487	C -3.450968 2.183838 0.113028
C 2.996973 -2.430199 -0.691003	C -2.815312 2.528290 0.160071	H -4.749382 0.481037 0.083006
H 3.942200 -1.240119 0.849548	H -4.301237 1.066202 0.648746	C -1.894962 4.144590 0.218958
H 4.404980 -0.784558 -0.761060	H -4.049648 1.267454 -1.055793	H 0.348476 3.325845 0.498073
C 1.547841 -2.874235 1.351888	C -0.806989 4.006953 0.260143	H 0.896342 2.257963 -0.777194
H 1.231843 -3.648965 -0.616353	H -0.082655 2.737059 -2.338811	H 0.942347 1.731590 0.903707
H -0.037421 -2.714602 -2.394619	H -1.439482 1.624379 -2.588772	H -4.258059 2.906963 0.163213
H 1.221412 -1.519031 -2.748567	H 0.215216 1.002245 -2.492970	H -1.255095 4.520621 -0.583729
H -0.435399 -0.995868 -2.463964	H -3.426718 3.358125 0.506539	H -1.426680 4.431795 1.165922
H 3.668538 -3.246234 -0.405306	H -0.287561 4.378485 -0.629970	H -2.850277 4.667882 0.155050
H 2.980400 -2.412787 -1.784768	H -0.043789 3.880049 1.036616	H 0.809682 -0.057202 -2.419045
H 0.544927 -3.150208 1.689339	H -1.508943 4.775555 0.590261	H 0.098651 -2.776310 -0.407518
H 1.824167 -1.947542 1.861243	H 1.050565 -1.541668 -2.187579	
H 2.241474 -3.656355 1.674956	H -0.194383 -3.039322 0.171101	
H -1.168993 1.472047 -2.203722		
H 0.008837 2.985128 0.207111		
E'-QH$_2$-G	**Eq'-QH$_2$-G**	**Eqn'-QH$_2$-G**
C 0.725719 1.908187 0.779586	C -0.842881 -1.980992 0.766689	C 0.047276 2.397771 0.226110
C 1.970695 2.412039 0.445330	C -2.098561 -2.435869 0.402326	C -1.322112 1.779065 0.057817
C 2.941926 1.547885 -0.070672	C -3.042723 -1.528633 -0.095079	H 0.044513 3.431928 -0.106634
C 2.681118 0.191608 -0.282227	C -2.741177 -0.173798 -0.235538	H 0.803065 1.876332 -0.358515
C 1.410005 -0.322735 0.035934	C -1.458679 0.287021 0.101767	H 0.377000 2.395251 1.267952
C 0.463684 0.557161 0.573163	C -0.536941 -0.631966 0.608935	C -1.539375 0.357984 0.151312
O 2.246621 3.736028 0.639722	O -2.411159 -3.758074 0.541287	C -2.394766 2.621054 -0.221392
O 4.153663 2.140203 -0.323253	O -4.257536 -2.086464 -0.403178	C -3.682420 2.081406 -0.447337
C 3.809706 -0.686808 -0.781163	C -3.800680 0.791740 -0.714247	C -2.851095 -0.164373 -0.142515
C 3.378319 -2.104810 -1.170175	C -3.508474 2.216440 -0.331880	C -0.558988 -0.613334 0.527076
C 2.328890 -2.667815 -0.205351	C -2.284964 2.658011 -0.040259	C -2.244697 4.123840 -0.298230
C 1.068344 -1.780715 -0.228943	C -1.087472 1.735829 -0.143174	C -3.908049 0.732650 -0.426251
C 0.283746 -1.926519 -1.546783	C -0.419701 1.892692 -1.531066	C -0.827163 -1.962289 0.551810
C 2.874602 -2.830687 1.218064	C -1.999836 4.080320 0.350338	H -4.505086 2.757712 -0.648914
N -3.753666 0.631279 -1.226901	N 3.639341 -0.639851 -1.280463	C -3.084472 -1.563640 -0.140738
C -4.653999 0.010594 -0.390403	C 4.562838 -0.074534 -0.429865	H -1.796765 4.536705 0.609038
N -4.319189 -0.521704 0.760149	N 4.258219 0.390413 0.757709	H -3.219887 4.593298 -0.432529
C -2.997775 -0.422112 1.066913	C 2.943408 0.281011 1.088274	H -1.613876 4.427490 -1.139156
C -2.035504 0.198907 0.267132	C 1.958619 -0.283618 0.274398	N 0.767466 -0.255138 0.945750
C -2.371369 0.782084 -0.986348	C 2.262456 -0.798296 -1.016590	C -2.088733 -2.453586 0.197438
N -2.415723 -0.911309 2.210087	N 2.391433 0.701515 2.272998	H -4.910449 0.362696 -0.603316
C -1.134135 -0.593353 2.103460	C 1.105563 0.398384 2.177512	H -0.051412 -2.658825 0.842752
N -0.834530 0.072917 0.954890	N 0.775198 -0.195345 0.997524	O -4.305840 -2.125536 -0.422151
O -1.653429 1.344011 -1.811951	O 1.522334 -1.311890 -1.854083	C 1.934233 -0.285241 0.194057
N -5.939015 -0.081135 -0.838505	N 5.837689 0.035957 -0.901551	C 1.148535 0.070484 2.210868
H -0.031514 2.559246 1.196591	H -0.107899 -2.670486 1.161015	H 0.424089 0.148382 3.007139

H 3.157065 3.902293 0.358077 H 4.574427 -0.738505 0.003950 H 4.294326 -0.221025 -1.647401 H 4.257413 -2.754125 -1.193833 H 2.970257 -2.095594 -2.183711 H 2.034048 -3.658324 -0.567809 H 0.413785 -2.129788 0.573551 H 0.049761 -2.978654 -1.731775 H 0.855297 -1.546846 -2.396362 H -0.654475 -1.372740 -1.508348 H 2.130162 -3.305133 1.863330 H 3.132085 -1.867268 1.666466 H 3.773267 -3.453880 1.222221 H -4.071540 0.997522 -2.116254 H -0.368671 -0.819503 2.830081 H -6.614794 -0.359038 -0.142319 H -6.272252 0.591609 -1.512696 H 4.767528 1.520031 -0.733051	H -3.317500 -3.891923 0.230386 H -4.774709 0.512685 -0.294756 H -3.916487 0.713965 -1.805423 H -4.354689 2.896083 -0.303584 H -0.355640 2.044741 0.607242 H -0.146631 2.934729 -1.712010 H -1.107754 1.574861 -2.318044 H 0.483463 1.285592 -1.600323 H -1.569231 4.123906 1.356924 H -2.905526 4.689303 0.335613 H -1.268097 4.537500 -0.324017 H 3.935158 -0.956918 -2.195918 H 0.358175 0.585777 2.933471 H 6.531583 0.268087 -0.206422 H 6.150017 -0.596770 -1.622904 H -4.841271 -1.450995 -0.832210	O -2.302674 -3.800284 0.208999 H -4.802267 -1.590145 -1.051728 C 2.179571 -0.519737 -1.186890 C 2.962601 0.054550 1.075107 N 2.451779 0.272795 2.331640 H -3.210749 -3.963157 -0.084509 N 4.273843 0.165114 0.733780 O 1.388982 -0.781982 -2.092013 N 3.560534 -0.403609 -1.450685 C 4.531209 -0.077515 -0.529539 H 3.825797 -0.580127 -2.412232 N 5.817756 -0.063488 -0.978627 H 6.486449 0.359551 -0.352317 H 5.996862 0.081080 -1.960927
E'-QH$_2$-A	**Eq'-QH$_2$-A**	**Eqn'-QH$_2$-A**
N -3.107085 0.976532 -1.647179 C -1.820485 1.084700 -1.426923 N -1.173465 0.691446 -0.301088 C -1.946931 0.149215 0.701246 C -3.336062 -0.003685 0.512603 C -3.910040 0.424312 -0.691242 N -1.582707 -0.290150 1.911084 C -2.780541 -0.705296 2.429539 N -3.860694 -0.564247 1.652731 H -2.838570 -1.126650 3.424533 N -5.218667 0.320666 -0.963672 H -5.854805 -0.050667 -0.276745 H -5.582721 0.676982 -1.833118 C 0.710151 2.153511 0.114694 C 2.071003 2.366800 0.261796 C 0.256161 0.868596 -0.161965 C 2.948127 1.283950 0.148909 O 2.538934 3.620869 0.531266 C 1.111744 -0.229242 -0.298457 C 2.490955 -0.007546 -0.131086 O 4.267871 1.599771 0.345500 H 3.501744 3.576195 0.614318 C 0.572404 -1.607379 -0.649711 C 3.503180 -1.132749 -0.180451 C 1.526751 -2.724552 -0.179716 C 0.270864 -1.712161 -2.157333 H -0.371239 -1.745589 -0.116588 C 2.940855 -2.456917 -0.707038 H 3.901188 -1.280034 0.831559 H 4.356659 -0.843209 -0.804594 C 1.497294 -2.890590 1.344186 H 1.172029 -3.659849 -0.625498 H -0.105272 -2.710525 -2.397080 H 1.163990 -1.528235 -2.758194 H -0.485964 -0.988701 -2.464354 H 3.611550 -3.271475 -0.421229 H 2.923677 -2.435592 -1.799467 H 0.494972 -3.166015 1.681826 H 1.773897 -1.966840 1.859331 H 2.190666 -3.674049 1.662974 H -1.190020 1.520335 -2.191821 H 0.015773 2.976487 0.223909 H 4.833752 0.826784 0.238676	N 3.001313 -1.131256 -1.626407 C 1.712682 -1.200218 -1.402612 N 1.081770 -0.786215 -0.274844 C 1.873830 -0.257962 0.721117 C 3.266052 -0.149059 0.529011 C 3.823318 -0.599849 -0.674740 N 1.524013 0.209578 1.925129 C 2.734351 0.595127 2.436322 N 3.809031 0.410571 1.660562 H 2.806937 1.028153 3.425344 N 5.133451 -0.536998 -0.950564 H 5.780785 -0.168406 -0.272652 H 5.483130 -0.892054 -1.826387 C -0.872401 -2.173782 0.106967 C -2.243635 -2.324286 0.235992 C -0.352230 -0.905937 -0.132816 C -3.071566 -1.198871 0.146469 O -2.772638 -3.562451 0.461345 C -1.157773 0.229297 -0.235922 C -2.542612 0.074411 -0.074399 O -4.407677 -1.464079 0.295060 H -3.732905 -3.475535 0.539830 C -0.578499 1.587328 -0.576595 C -3.457450 1.276615 -0.108835 C -1.422202 2.722167 -0.032971 C -0.416693 1.734803 -2.109317 H 0.414981 1.667360 -0.130468 C -2.734346 2.570120 0.145792 H -4.244226 1.168234 0.648283 H -3.983207 1.322872 -1.073857 C -0.703396 4.012765 0.239790 H -0.004295 2.714359 -2.361294 H -1.384933 1.630408 -2.604358 H 0.256750 0.973421 -2.508402 H -3.337399 3.403818 0.492352 H -0.179301 4.371718 -0.652303 H 0.057359 3.871249 1.015435 H -1.391709 4.793206 0.569023 H 1.067075 -1.618153 -2.164891 H -0.221598 -3.033962 0.195456 H -4.936544 -0.660207 0.240997	N 2.844422 0.104395 -1.927077 C 1.585062 -0.123420 -1.651220 N 1.085796 -0.414582 -0.424338 C 1.988527 -0.507374 0.609624 C 3.357564 -0.270765 0.370218 C 3.775201 0.045377 -0.929130 N 1.771549 -0.770835 1.902651 C 3.038631 -0.691521 2.419047 N 4.025294 -0.398246 1.564712 H 3.220314 -0.861038 3.472069 N 5.050146 0.296374 -1.255199 H 5.772357 0.264861 -0.553825 H 5.293025 0.521291 -2.207020 C -0.668326 -2.011347 -0.308200 C -2.004245 -2.413253 -0.197826 C -0.324725 -0.681708 -0.245839 C -2.985064 -1.453866 -0.067161 O -2.300894 -3.743035 -0.240025 C -1.287853 0.358894 -0.068332 C -2.663536 -0.072558 -0.030028 O -4.270162 -1.931926 -0.022599 H -3.257064 -3.843374 -0.126759 C -0.996982 1.764237 0.057552 C -3.691825 0.897094 0.035746 C -2.043871 2.679262 0.113976 C 0.417766 2.286501 0.170400 C -3.384337 2.228594 0.087344 H -4.732594 0.598150 0.019209 C -1.810161 4.169922 0.210334 H 0.417847 3.323340 0.494449 H 0.953447 2.251130 -0.781624 H 0.996602 1.725104 0.902251 H -4.183255 2.960375 0.118579 H -1.160870 4.534240 -0.589503 H -1.343223 4.447524 1.160186 H -2.757911 4.704897 0.141308 H 0.852257 -0.074890 -2.446917 H 0.099401 -2.762074 -0.444546 H -4.853287 -1.334002 0.458868
E'-QH$_2$-GH$^+$	**Eq'-QH$_2$-GH$^+$**	**Eqn'-QH$_2$-GH$^+$**
C 0.722690 1.883087 0.815297 C 1.957121 2.413524 0.484657 C 2.941997 1.573232 -0.047004 C 2.705802 0.215451 -0.277574 C 1.445715 -0.327757 0.036470 C 0.489772 0.530435 0.588676 O 2.209057 3.737773 0.696582	C -0.839399 -1.965534 0.792263 C -2.085968 -2.445103 0.429809 C -3.044302 -1.558055 -0.079342 C -2.766720 -0.199522 -0.233241 C -1.493838 0.288437 0.102326 C -0.561886 -0.612502 0.620223 O -2.375545 -3.769341 0.581365	C 0.005510 2.409511 0.220664 C -1.359798 1.782175 0.049866 H -0.002963 3.442952 -0.113263 H 0.765905 1.896929 -0.365995 H 0.333212 2.413829 1.263069 C -1.571015 0.360800 0.149429 C -2.435185 2.617400 -0.237359

O 4.139289 2.191242 -0.295491	O -4.245501 -2.140275 -0.385960	C -3.719466 2.070398 -0.465105
C 3.848189 -0.633776 -0.794470	C -3.841038 0.741704 -0.726344	C -2.879494 -0.170045 -0.144354
C 3.442081 -2.053433 -1.203858	C -3.575812 2.175106 -0.357590	C -0.591430 -0.607786 0.529381
C 2.406440 -2.650367 -0.244823	C -2.361524 2.641940 -0.067653	C -2.292271 4.120208 -0.322280
C 1.129164 -1.786910 -0.252283	C -1.147186 1.740419 -0.159409	C -3.938837 0.721186 -0.436761
C 0.346214 -1.924062 -1.572129	C -0.482047 1.892464 -1.549012	C -0.849617 -1.958562 0.560515
C 2.958366 -2.823683 1.174941	C -2.102218 4.072373 0.310532	H -4.544318 2.741479 -0.674159
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C -4.667746 0.053496 -0.462779	C 4.577791 -0.102489 -0.502081	H -1.850781 4.540402 0.584692
N -4.267768 -0.534001 0.679008	N 4.206391 0.403231 0.687471	H -3.269024 4.583872 -0.463999
C -2.939292 -0.474357 1.048875	C 2.885955 0.323204 1.081418	H -1.659119 4.421395 -1.162263
C -2.000944 0.175655 0.269395	C 1.926625 -0.263401 0.277660	N 0.737530 -0.245008 0.951353
C -2.336766 0.812685 -0.963148	C 2.232393 -0.814347 -1.003173	C -2.108266 -2.456222 0.208983
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C -1.106342 -0.687170 2.076627	C 1.076996 0.473602 2.161398	H -0.072075 -2.650498 0.857347
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H 3.115226 3.926176 0.414689	H -3.279702 -3.923056 0.272958	O -2.316733 -3.802656 0.228796
H 4.616643 -0.682656 -0.012955	H -4.811708 0.449931 -0.307839	H -4.849415 -1.583739 -0.997840
H 4.319798 -0.145157 -1.655088	H -3.950275 0.650071 -1.816976	C 2.149815 -0.543134 -1.184890
H 4.332962 -2.685679 -1.239076	H -4.434357 2.839173 -0.337595	C 2.901361 0.067461 1.079986
H 3.031465 -2.036799 -2.216200	H -0.422871 2.073938 0.587670	N 2.427662 0.302354 2.321535
H 2.128516 -3.640410 -0.621108	H -0.234184 2.937853 -1.744816	H -3.224063 -3.973498 -0.062226
H 0.483939 -2.164673 0.544672	H -1.160477 1.545630 -2.331714	N 4.217931 0.156185 0.677719
H 0.140832 -2.977541 -1.780378	H 0.437492 1.309066 -1.611010	O 1.379262 -0.822754 -2.080476
H 0.904644 -1.508823 -2.413418	H -1.675693 4.132609 1.317977	N 3.550919 -0.422758 -1.464959
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H 2.224300 -3.320647 1.815042	H -1.376754 4.536294 -0.365945	H 3.793541 -0.591951 -2.434926
H 3.200249 -1.862610 1.636854	H 3.915044 -1.051220 -2.178945	N 5.796785 -0.006353 -1.017747
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H -4.045718 1.118631 -2.084307	H 6.561012 0.357175 -0.329569	H 6.048709 -0.199452 -1.975277
H -0.350988 -0.943569 2.802373	H 6.118390 -0.434628 -1.794661	H 4.931183 0.406994 1.351656
H -6.641457 -0.441284 -0.284941	H -4.846563 -1.516336 -0.808280	
H -6.238925 0.468516 -1.693145	H 4.882537 0.850143 1.295020	
H 4.766751 1.588591 -0.711104		
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E'-QH_2-AH^+	**Eq'-QH_2-AH^+**	**Eqn'-QH_2-AH^+**
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C -1.830541 0.935085 -1.499747	C 1.702327 -1.219959 -1.414598	C 1.562414 -0.062517 -1.669939
N -1.183375 0.579193 -0.362258	N 1.066752 -0.781890 -0.298885	N 1.068745 -0.378640 -0.447209
C -1.967595 0.095726 0.651192	C 1.856522 -0.242990 0.681744	C 1.977242 -0.490681 0.569595
C -3.349961 -0.027143 0.475516	C 3.235447 -0.144328 0.495266	C 3.330931 -0.255059 0.328514
C -3.939050 0.358447 -0.744245	C 3.821113 -0.619043 -0.695258	C 3.764271 0.095445 -0.966068
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C -2.692483 -0.657217 2.481638	C 2.600543 0.649168 2.446332	C 2.934126 -0.752211 2.434417
N -3.795495 -0.522347 1.689822	N 3.687378 0.440734 1.662135	N 3.923827 -0.434283 1.563339
H -2.759046 -1.026443 3.494688	H 2.680000 1.098896 3.423478	H 3.132824 -0.945543 3.476834
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H -5.939792 -0.047283 -0.392250	H 5.808100 -0.201105 -0.351627	H 5.785691 0.323855 -0.656221
H -5.546702 0.609857 -1.945851	H 5.433972 -0.953802 -1.865390	H 5.222447 0.596597 -2.271528
C 0.619899 2.131237 0.063199	C -0.874876 -2.176849 0.108408	C -0.661427 -2.001448 -0.333114
C 1.961744 2.429125 0.235531	C -2.243772 -2.332420 0.251580	C -1.990060 -2.422732 -0.221601
C 0.250657 0.815643 -0.204377	C -0.368812 -0.906017 -0.144035	C -0.340625 -0.666463 -0.259344
C 2.899171 1.389910 0.156167	C -3.077278 -1.209495 0.165181	C -2.984086 -1.476941 -0.079152
O 2.338048 3.702416 0.495080	O -2.764070 -3.569434 0.489302	O -2.267537 -3.755021 -0.275527
C 1.162224 -0.240586 -0.313832	C -1.176257 0.226691 -0.248409	C -1.313301 0.361253 -0.069688
C 2.523373 0.070258 -0.116862	C -2.558189 0.065059 -0.069791	C -2.682114 -0.091448 -0.029900
O 4.187106 1.786441 0.382528	O -4.407345 -1.479860 0.339346	O -4.257627 -1.976042 -0.031237
H 3.299245 3.734586 0.598554	H -3.725903 -3.490501 0.559687	H -3.221748 -3.872639 -0.162752
C 0.719309 -1.659031 -0.661618	C -0.608798 1.584408 -0.609750	C -1.041756 1.768679 0.069239
C 3.603881 -0.994664 -0.120991	C -3.479188 1.261972 -0.101275	C -3.723322 0.863184 0.049920
C 1.728968 -2.716111 -0.151647	C -1.451010 2.718729 -0.062690	C -2.100984 2.667899 0.137782
C 0.456789 -1.811261 -2.175921	C -0.470180 1.717450 -2.145547	C 0.365533 2.310991 0.183060
H -0.226723 -1.855591 -0.145691	H 0.390693 1.679655 -0.179907	C -3.434993 2.198053 0.112467
C 3.142207 -2.362775 -0.638073	C -2.759496 2.560521 0.134800	H -4.760468 0.551601 0.036813
H 3.984050 -1.099346 0.903869	H -4.255667 1.152783 0.665310	C -1.888491 4.160462 0.247743
H 4.455194 -0.664533 -0.730399	H -4.015227 1.298858 -1.060891	H 0.350624 3.344694 0.515847
C 1.657602 -2.895904 1.371788	C -0.734882 4.014679 0.190650	H 0.900730 2.295928 -0.769756
H 1.450265 -3.670936 -0.610776	H -0.069368 2.697606 -2.412228	H 0.954593 1.758294 0.913450

H 0.138669 -2.831946 -2.405378 H 1.349510 -1.593795 -2.765562 H -0.329182 -1.136851 -2.524706 H 3.853093 -3.128485 -0.316518 H 3.164499 -2.365518 -1.731158 H 0.665006 -3.240178 1.675296 H 1.856694 -1.965202 1.909876 H 2.382663 -3.641649 1.708989 H -1.201969 1.333993 -2.286816 H -0.114857 2.921468 0.154846 H 4.809495 1.058109 0.283914 H -4.741817 -0.742452 1.964539	H -1.444794 1.600413 -2.624438 H 0.203008 0.958217 -2.549300 H -3.362470 3.393417 0.482827 H 0.035713 3.883439 0.958394 H -1.423203 4.794146 0.521760 H -0.223610 4.368737 -0.710605 H 1.060992 -1.649029 -2.173889 H -0.218605 -3.032779 0.195928 H -4.950645 -0.692814 0.218805 H 4.639013 0.676285 1.908585	H -4.244095 2.917737 0.154551 H -1.423043 4.434948 1.199183 H -2.843980 4.682201 0.186679 H -1.247015 4.541506 -0.550474 H 0.827797 0.000911 -2.462625 H 0.115162 -2.740613 -0.481500 H -4.863053 -1.368894 0.409212 H 4.903392 -0.355024 1.800202