Metal-Free Catalytic Conversion of CO_2 Into Methanol: Local Electrophilicity as a Tuning Property in the Design and Performance of the Aniline-Derived Aminoborane-Based FLPs

Electronic Supplementary Information (ESI)

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1. Energetic analysis

Table S1. Activation Gibbs free energy (ΔG_{act}) and Gibbs free energy change (ΔG^o) at 353 K (80ºC), associated with the H_2 activation and all hydrogenation processes in **gas-phase**. The ZPE corrected electronic energy values are shown in parenthesis. All values are in kcal/mol.

FLP	H_2		CO_2		HCOOH		$CH_2(OH)_2$		CH_2O	
	ΔG_{act}	ΔG^o	ΔG_{act}	ΔG^o	ΔG_{act}	ΔG^o	ΔG_{act}	ΔG^o	ΔG_{act}	ΔG^o
Mes	23.6 (14.1)	17.3 (7.4)	23.4 (10.3)	-2.3 (1.2)	24.0 (8.1)	-12.4 (-10.7)	59.0 (43.5)	-30.4 (-17.0)	16.6 (2.0)	-30.7 (-28.8)
Mes'	23.2 (13.2)	16.0 (5.8)	20.4 (7.0)	-1.9 (2.8)	20.5 (4.9)	-11.9 (-9.2)	46.5 (32.0)	-29.9 (-15.5)	14.4 (-0.1)	-30.2 (-27.3)
H	15.0 (6.0)	10.5 (7.4)	18.8 (6.0)	4.4 (6.8)	18.6 (3.2)	-12.4 (-5.2)	59.5 (44.9)	-23.7 (-11.5)	10.5 (-3.8)	-23.9 (-23.3)
FMes	28.6 (19.4)	8.3 (-1.6)	38.8 (26.1)	6.6 (10.2)	37.0 (21.0)	-3.5 (-1.7)	54.8 (39.6)	-21.5 (-8.1)	21.2 (6.0)	-21.7 (-19.8)
CF_3	13.3 (4.7)	-12.4 (-21.7)	41.4 (28.2)	27.4 (30.3)	32.2 (16.5)	17.3 (18.3)	43.3 (28.3)	-0.7 (12.0)	19.0 (4.5)	-1.0 (0.2)
PFtb	19.1 (10.4)	-23.8 (-32.7)	58.5 (44.7)	38.8 (41.3)	51.5 (37.2)	28.7 (29.3)	63.1 (47.6)	10.7 (23.0)	30.9 (15.7)	10.4 (11.2)
C_6F_5	19.9 (11.1)	2.3 (-6.7)	32.2 (18.6)	12.7 (15.3)	25.5 (9.5)	2.6 (3.3)	50.0 (35.1)	-15.4 (-3.0)	16.4 (1.3)	-15.7 (-14.8)

Table S2. Activation Gibbs free energy (ΔG_{act}) and Gibbs free energy change (ΔG^o) at 353 K (80ºC), associated with the H_2 activation and all hydrogenation processes in **benzene**. The ZPE corrected electronic energy values are shown in parenthesis. All values are in kcal/mol.

FLP	H_2		CO_2		HCOOH		$CH_2(OH)_2$		CH_2O	
	ΔG_{act}	ΔG^o	ΔG_{act}	ΔG^o	ΔG_{act}	ΔG^o	ΔG_{act}	ΔG^o	ΔG_{act}	ΔG^o
Mes	23.2 (13.7)	13.1 (3.2)	22.9 (9.8)	-2.2 (1.4)	27.6 (11.7)	-9.0 (-7.3)	63.1 (47.7)	-28.0 (-14.7)	19.3 (4.6)	-24.7 (-25.4)
Mes'	22.2 (12.2)	12.3 (2.1)	20.3 (6.9)	-1.3 (2.5)	23.4 (7.8)	-8.2 (-6.2)	51.0 (36.4)	-27.2 (-13.6)	16.4 (1.9)	-23.0 (-24.3)
H	13.6 (4.7)	4.3 (-4.4)	19.9 (7.1)	6.6 (9.0)	23.3 (7.9)	-0.2 (0.3)	61.7 (47.0)	-19.2 (-7.0)	14.2 (-0.1)	-21.5 (-17.8)
FMes	28.4 (19.2)	3.7 (-6.3)	39.7 (27.0)	7.2 (10.9)	44.8 (28.8)	0.4 (2.1)	59.5 (44.3)	-18.6 (-5.2)	24.8 (9.5)	-14.2 (-15.9)
CF_3	13.4 (4.7)	-18.2 (-27.5)	44.8 (31.6)	29.1 (32.1)	37.9 (22.2)	22.3 (23.4)	49.7 (34.8)	-3.3 (16.1)	23.0 (8.5)	5.9 (5.3)
PFtb	18.8 (10.1)	-30.1 (-39.1)	61.9 (48.1)	41.0 (43.6)	58.1 (42.1)	34.2 (34.9)	67.8 (52.4)	15.2 (27.6)	36.0 (20.7)	17.4 (16.9)
C_6F_5	19.7 (11.0)	-2.4 (-11.3)	32.7 (19.1)	13.3 (15.9)	29.6 (13.6)	6.5 (7.2)	54.9 (39.9)	-12.5 (-0.2)	19.0 (3.9)	-11.8 (-10.9)

2. Side reactions

Table S3. Activation Gibbs free energy (ΔG_{act}) and Gibbs free energy change (ΔG^o) at 353 K (80ºC), associated with the protodeborylation of the FLPs in gas-phase and benzene. Enthalpies are shown in parenthesis. All values are in kcal/mol.

FLP	ΔG_{act} (ΔH_{act})	ΔG^o (ΔH^o)
Gas-phase		
Mes	14.0 (14.3)	-25.4 (-3.4)
Mes'	10.3 (10.3)	-23.6 (-3.9)
C6F5	20.3 (20.1)	-9.0 (8.1)
Benzene		
Mes	16.4 (16.7)	-25.3 (-3.3)
Mes'	12.6 (12.7)	-23.0 (-3.3)
C6F5	23.6 (23.4)	-7.6 (9.5)

Table S4. Gibbs free energy change (ΔG^o) at 353 K (80ºC), associated with the dimerisation of the FLPs after the first protodeborylation into an 8-membered ring boat-type structure and into a diborane-type structure in gas phase and benzene. Enthalpies are shown in parenthesis. All values are in kcal/mol.

FLP	8-member ring dimer	Diborane dimer
Gas-phase		
Mes	36.4 (9.1)	-0.2 (-24.3)
Mes'	22.1 (-2.4)	-0.1 (-20.2)
C6F5	7.6 (-17.9)	-6.8 (-28.4)
Benzene		
Mes	39.1 (11.9)	5.0 (-19.2)
Mes'	24.4 (-0.1)	4.2 (-15.9)

C6F5	14.2 (-10.4)	0.4 (-20.3)

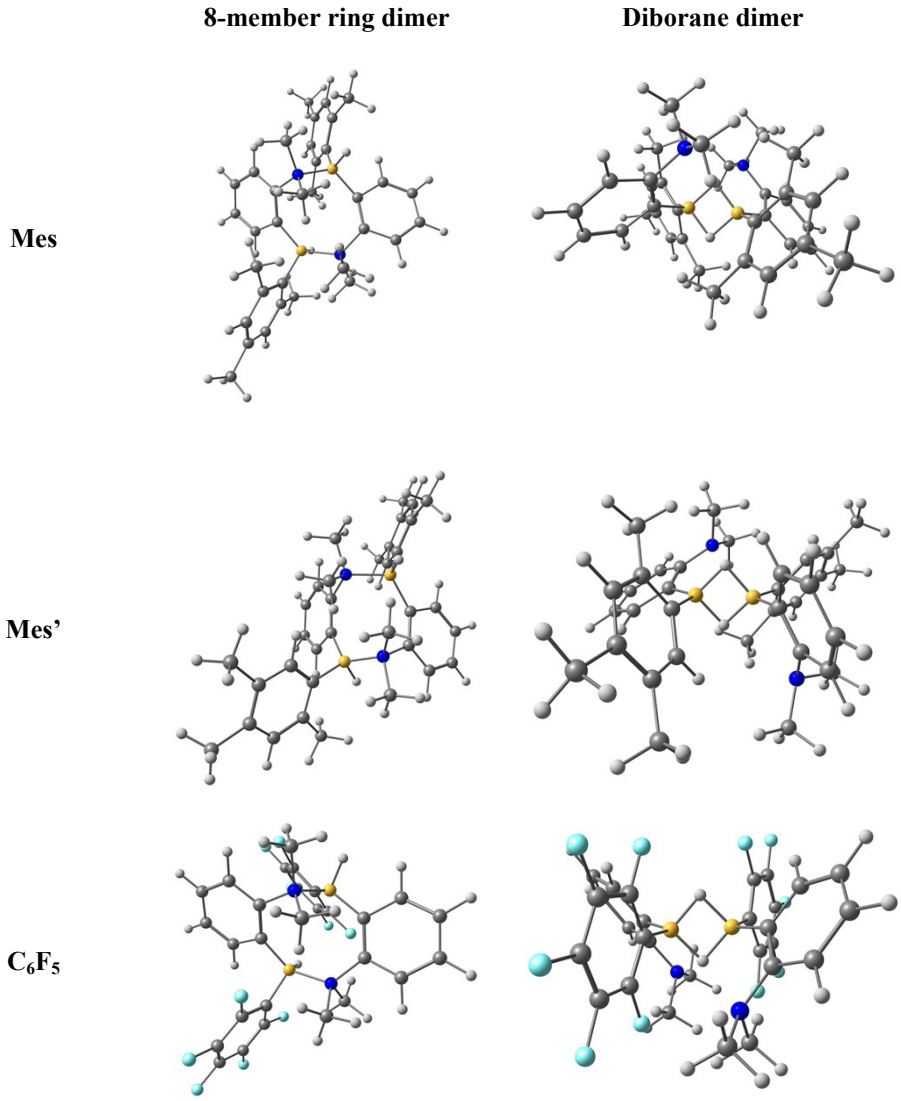

Figure S1. Structures of the 8-member ring and diborane dimers with **Mes**, **Mes'** and **C_6F_5**.

3. Mechanistic analysis

Table S5. Activation energy (ΔE_{act}), total distortion energy (ΔE_{dist}) and the components associated with each reactant and interaction energy (ΔE_{int}) of the **CO2 and HCOOH hydrogenation** processes. All values are in kcal/mol.

FLP	CO_2					HCOOH				
	ΔE_{act}	ΔE_{dist} FLP	ΔE_{dist} CO2	ΔE_{dist}	ΔE_{int}	ΔE_{act}	ΔE_{dist} FLP	ΔE_{dist} HCOOH	ΔE_{dist}	ΔE_{int}
Mes	9.7	16.6 (33%)	33.2 (67%)	49.8	-40.1	12.5	24.2 (60%)	16.4 (40%)	40.6	-28.0
Mes'	7.2	18.5 (32%)	38.8 (68%)	57.3	-50.1	9.0	20.2 (57%)	15.2 (43%)	35.4	-26.4
H	6.4	9.3 (25%)	27.7 (75%)	37.0	-30.6	8.0	16.8 (48%)	18.0 (52%)	34.8	-26.9
FMes	29.8	49.2 (51%)	47.2 (49%)	96.4	-66.6	31.9	46.3 (67%)	23.0 (33%)	69.2	-37.4
CF_3	33.7	60.6 (55%)	50.1 (45%)	110.7	-77.0	24.1	47.4 (69%)	21.4 (31%)	68.8	-44.8
PFtb	49.8	84.6 (60%)	56.8 (40%)	141.3	-91.9	42.3	115.7 (72%)	45.1 (28%)	160.8	-118.6
C_6F_5	21.0	37.7 (45%)	45.4 (55%)	83.1	-62.1	15.8	31.5 (62%)	19.5 (38%)	51.0	-35.2

Table S6. Activation energy (ΔE_{act}), total distortion energy (ΔE_{dist}) and the components associated with each reactant and interaction energy (ΔE_{int}) of the **methanediol and formaldehyde hydrogenation** processes. All values are in kcal/mol.

FLP	$CH_2(OH)_2$					CH_2O				
	ΔE_{act}	ΔE_{dist} FLP	ΔE_{dist} CO2	ΔE_{dist}	ΔE_{int}	ΔE_{act}	ΔE_{dist} FLP	ΔE_{dist} HCOOH	ΔE_{dist}	ΔE_{int}
Mes	49.3	94.0 (52%)	88.2 (48%)	182.2	-132.9	3.4	15.1 (70%)	6.5 (30%)	21.6	-18.2
Mes'	39.5	100.6 (50%)	100.4 (50%)	201.0	-161.5	0.8	12.5 (67%)	6.0 (33%)	18.5	-17.7
H	49.3	73.5 (49%)	75.1 (51%)	148.7	-100.5	-2.3	8.5 (59%)	5.8 (41%)	14.2	-16.5
FMes	46.8	89.4 (46%)	107.0 (54%)	196.4	-149.6	9.8	23.4 (68%)	10.8 (32%)	34.2	-24.4
CF_3	37.5	97.6 (48%)	105.9 (52%)	203.5	-166.0	9.4	18.9 (61%)	12.2 (39%)	31.1	-21.8
PFtb	54.6	104.8 (50%)	104.6 (50%)	209.5	-154.8	21.5	49.4 (79%)	13.1 (21%)	62.5	-41.0
C_6F_5	42.7	98.0 (49%)	103.0 (51%)	200.9	-158.2	2.9	14.3 (65%)	7.6 (35%)	21.9	-18.9

Table S7. Internuclear distances B-H and N-H at TS for each hydrogenation. All values are in Å.

FLP	CO_2		HCOOH		$CH_2(OH)_2$		CH_2O	
	d_{B-H}	d_{N-H}	d_{B-H}	d_{N-H}	d_{B-H}	d_{N-H}	d_{B-H}	d_{N-H}
Mes	1.423	1.056	1.349	1.137	1.247	1.749	1.320	1.056
Mes'	1.448	1.074	1.311	1.128	1.234	1.810	1.301	1.049
H	1.330	1.067	1.314	1.155	1.236	1.640	1.281	1.062
FMes	1.557	1.262	1.399	1.328	1.243	1.763	1.328	1.185
CF_3	1.506	1.423	1.309	1.405	1.221	1.815	1.309	1.173
PFtb	1.775	1.421	1.835	1.653	1.228	1.774	1.336	1.344
C_6F_5	1.531	1.202	1.326	1.272	1.238	1.800	1.280	1.099

Table S8. Variation of the internuclear distances B-H and N-H ($\Delta d = d_{TS} - d_R$). All values are in Å.

FLP	CO_2		HCOOH		$CH_2(OH)_2$		CH_2O	
	Δd_{B-H}	Δd_{N-H}	Δd_{B-H}	Δd_{N-H}	Δd_{B-H}	Δd_{N-H}	Δd_{B-H}	Δd_{N-H}
Mes	**0.074**	-0.002	0.059	**0.086**	-0.019	**0.571**	**0.025**	-0.007
Mes'	**0.203**	0.037	0.066	**0.090**	-0.012	**0.773**	**0.055**	0.011
H	**0.187**	0.019	**0.113**	0.100	0.011	**0.712**	**0.084**	0.018
FMes	**0.347**	0.230	0.189	**0.296**	0.033	**0.731**	0.118	**0.153**
CF_3	0.285	**0.391**	0.087	**0.373**	-0.001	**0.783**	0.087	**0.141**
PFtb	**0.563**	0.388	**0.725**	0.704	0.015	**0.741**	0.124	**0.311**
C_6F_5	**0.303**	0.161	0.098	**0.231**	0.010	**0.758**	0.052	**0.058**

Table S9. Internuclear distances of B-H and N-H of catalyst, C-O of methanediol, and O-H and C-H of methanediol-catalyst at TS structure of methanediol hydrogenation. All values are in Å.

FLP	B-H	N-H	C-O	O-H	C-H
Mes	1.234	1.810	2.611	0.991	2.257
Mes'	1.247	1.749	2.417	0.999	2.092
H	1.236	1.640	2.258	1.024	2.259
FMes	1.243	1.763	2.570	0.997	2.333
CF_3	1.221	1.815	2.616	0.992	2.226
PFtb	1.228	1.774	2.603	0.994	2.204
C_6F_5	1.238	1.800	2.615	0.994	2.132

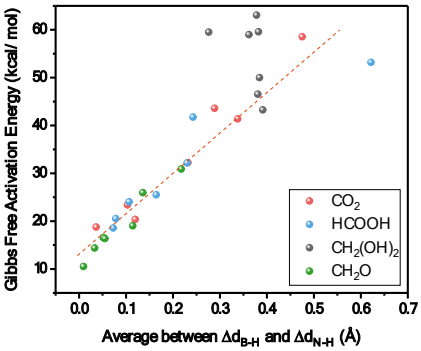

Figure S2. Relation between activation energy and the variation of the internuclear distances B-H and N-H ($\Delta d = d_{TS} - d_R$). The linear relationship shown corresponds to the relation considering CO_2, HCOOH and CH_2O hydrogenations with a linear fit equation of $\Delta G_{act} = 80.2\Delta d + 13.8$; $R^2 = 0.90$.

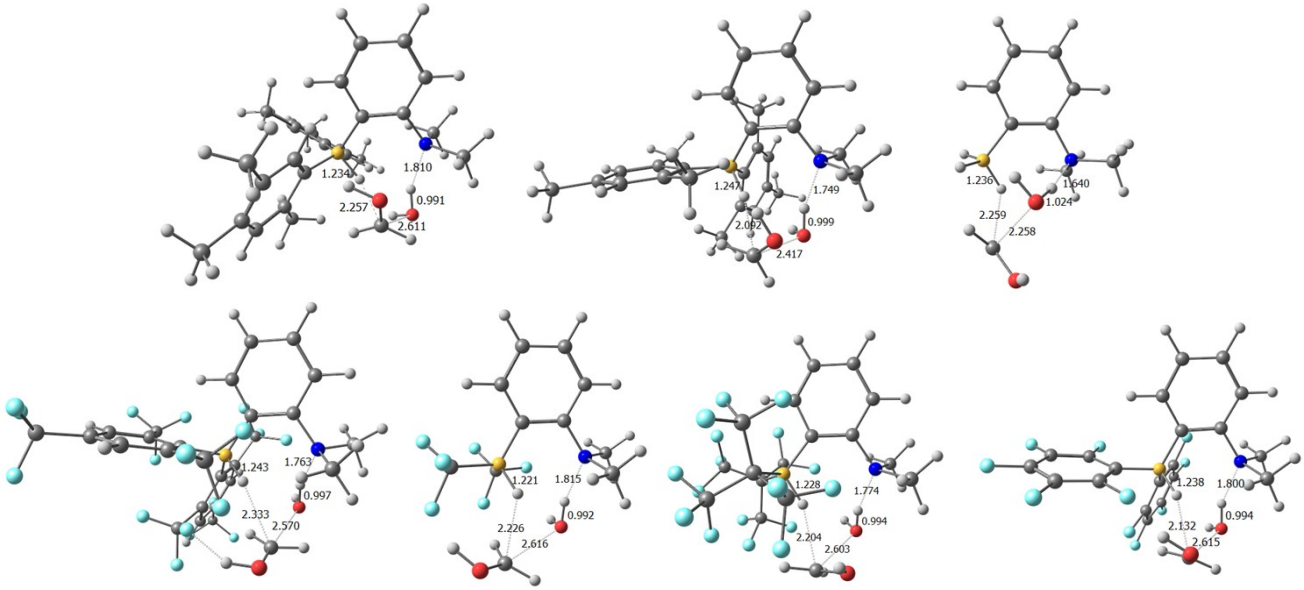

Figure S3. Transition state structures of the methanediol hydrogenation.

Table S10. Gibbs free energy obtained from the linear fit equation between ΔG_{act} and ω_B ($\beta\omega_B + \alpha$) and the energy associated to steric effect (ΔE_{steric}).

FLP	CO_2		HCOOH		CH_2O	
	$\beta\omega_B + \alpha$	ΔE_{steric}	$\beta\omega_B + \alpha$	ΔE_{steric}	$\beta\omega_B + \alpha$	ΔE_{steric}
Mes	20.4	2.4	20.8	6.8	12.9	6.3
Mes'	16.9	3.4	17.7	5.7	11.1	5.3
H	21.5	-1.7	21.7	1.6	13.5	0.7
FMes	28.1	11.6	27.3	17.5	17.0	7.8
CF_3	42.5	2.2	39.5	-1.6	24.5	-1.5
PFtb	63.2	-1.3	57.0	1.0	35.3	0.6
C_6F_5	32.1	0.7	30.6	-1.0	19.0	0.0

4. Activation Strain Model analysis of methanediol hydrogenation

As we have seen, the mehtanediol is the limiting step, showing gibbs free energies that range from 49.7 to 69.8 kcal/mol, which avoids the methanol formation following this mechanism. Moreover, we have seen that exists a correlation between the activation energy and the interaction energy between the fragments in some cases and with the distortion energy in others. For that reason, we have analysed the mechanism of this kinetic step in detail, employing the Activation Strain Model of reactivity (*Angew. Chem. Int. Ed.* 2017, 56, 10070–10086) to analyse the main factors that are governing the activation free energy of these reactions. Fig S4 shows the ASM profile for all reactions, where it can be seen that the reaction is dominated by the strain energy, which we have decomposed it in terms of the strain of both reagents and we have found that the strain of both in similar extent are dominating the activation energy of this process. Another interesting result is that the interaction energy between the fragments is always negative, i.e., it is attractive from the beginning of the reaction.

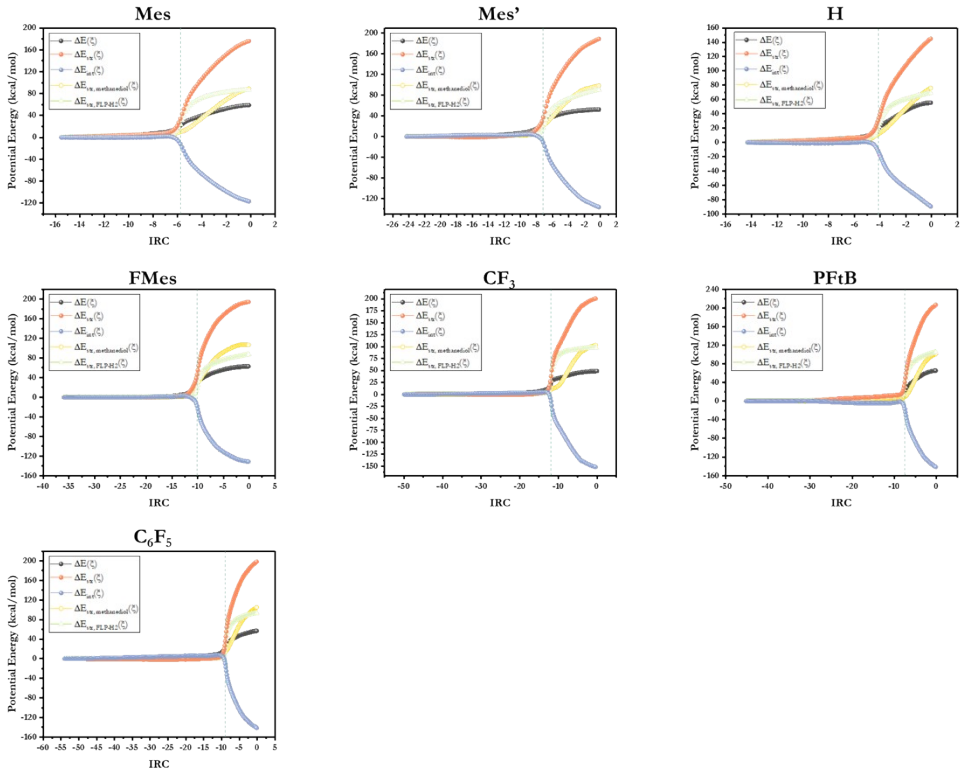

Figure S4. ASM diagrams of the methanediol hydrogenation employing the seven catalysts analysed in this work. The total, strain and interaction energies are represented by the black, red and blue lines respectively. The strain energy was partitioned in terms of the strain of methanediol and the catalyst, which are depicted in yellow and green lines, respectively.

5. Analysis of catalytic activity

Table S11. Absolute TOF values for methanol formation and all the intermediates of the catalytic cycle, obtained from ESM in h^{-1} employing the **ZPE corrected electronic energy** at 353 K.

FLP	TOF HCOOH	TOF Methanediol	TOF Methanol from methanediol	TOF Methanol from formaldehyde
Mes	$1.0x10^{7}$	$2.0x10^{4}$	$3.0x10^{-16}$	$1.2x10^{4}$
Mes'	$2.0x10^{7}$	$1.0x10^{6}$	$1.2x10^{-8}$	$8.8x10^{5}$
H	$8.9x10^{7}$	$7.7x10^{7}$	$6.9x10^{-14}$	$7.5x10^{7}$
FMes	$6.2x10^{-3}$	$5.8x10^{-5}$	$3.5x10^{-12}$	$5.8x10^{-5}$
CF_3	$4.0x10^{-7}$	$4.1x10^{-7}$	$3.5x10^{-7}$	$4.1x10^{-7}$
PFtB	$1.2x10^{-22}$	$1.3x10^{-17}$	$9.6x10^{-18}$	$1.3x10^{-17}$
C_6F_5	$6.0x10^{-1}$	$6.1x10^{-1}$	$1.8x10^{-9}$	$6.1x10^{-1}$

Table S12. Absolute TOF values for methanol formation and all the intermediates of the catalytic cycle, obtained from ESM in h^{-1} employing the **Gibbs free energy** at 353 K.

FLP	TOF HCOOH	TOF Methanediol	TOF Methanol from methanediol	TOF Methanol from formaldehyde
Mes	$1.4x10^{-6}$	$2.8x10^{-16}$	$8.6x10^{-41}$	$2.8x10^{-16}$
Mes'	$1.8x10^{-4}$	$3.4x10^{-13}$	$8.4x10^{-33}$	$3.4x10^{-13}$
H	$2.9x10^{1}$	$3.8x10^{-8}$	$1.8x10^{-34}$	$3.8x10^{-8}$
FMes	$3.4x10^{-11}$	$4.4x10^{-21}$	$1.0x10^{-32}$	$4.4x10^{-21}$
CF_3	$5.0x10^{-12}$	$7.7x10^{-15}$	$2.3x10^{-24}$	$1.6x10^{-14}$
PFtB	$1.2x10^{-22}$	$5.0x10^{-27}$	$1.4x10^{-35}$	$5.1x10^{-27}$
C_6F_5	$5.8x10^{-5}$	$1.9x10^{-9}$	$1.4x10^{-27}$	$1.9x10^{-9}$

Table S13. Control degree of TSs and Is obtained with **ΔG** and **ΔE+ZPE**, shown in parenthesis, for **methanol formation from methanediol hydrogenation.**

X_{TOF}	H	Mes'	Mes	FMes	CF_3	PFtB	C_6F_5
TS1	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)
TS2	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)
TS3	0 (0)	0 (0)	0 (0)	0 (0)	0 (**0.9**)	0 (**0.7**)	0 (0)
TS4	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)
TS5	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)
TS6	**1** (**1**)	**1** (**1**)	**1** (**1**)	**1** (**1**)	**1** (**0.1**)	**1** (**0.3**)	**1** (**1**)
I0	**1** (0)	**1** (**0.7**)	**1** (**0.7**)	**1** (0)	0 (0)	0 (0)	0 (0)
I1	0 (**0.6**)	0 (0)	0 (0)	0 (**0.6**)	**1** (0)	**1** (**0.9**)	**1** (**0.6**)
I2	0 (0)	0 (0)	0 (0)	0 (0)	0 (**1**)	0 (0)	0 (0)
I3	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)
I4	0 (0)	0 (**0.3**)	0 (**0.3**)	0 (0)	0 (0)	0 (0)	0 (0)
I5	0 (**0.4**)	0 (0)	0 (0)	0 (**0.4**)	0 (0)	0 (**0.1**)	0 (**0.4**)

Table S14. Control degree of TSs and Is obtained with **ΔG** and **ΔE+ZPE**, shown in parenthesis, for **methanol formation from formaldehyde hydrogenation**.

X_{TOF}	H	Mes'	Mes	FMes	CF_3	PFtB	C_6F_5
TS1	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)
TS2	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)
TS3	0 (**0.8**)	0 (**0.9**)	0 (**0.1**)	0 (0)	0 (**1**)	0 (**1**)	0 (**1**)
TS4	**1** (**0.2**)	**1** (0)	**1** (**0.5**)	**1** (**1**)	**1** (0)	**1** (0)	**1** (0)
TS5	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)
TS6	0 (0)	0 (**0.1**)	0 (**0.4**)	0 (0)	0 (0)	0 (0)	0 (0)
I0	**1** (0)	**1** (**0.9**)	**1** (**0.9**)	**1** (0)	0 (0)	0 (0)	0 (0)
I1	0 (**1**)	0 (**0.1**)	0 (0)	0 (**1**)	**1** (**1**)	**1** (**1**)	**1** (**1**)
I2	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)
I3	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)
I4	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)
I5	0 (0)	0 (0)	0 (**0.1**)	0 (0)	0 (0)	0 (0)	0 (0)

Table S15. Control degree of TSs and Is obtained with **ΔG** and **ΔE+ZPE**, shown in parenthesis, for **methanediol formation**.

X_{TOF}	H	Mes'	Mes	FMes	CF_3	PFtB	C_6F_5
TS1	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)
TS2	0 (0)	0 (0)	0 (0)	0 (0)	**0.5** (0)	0 (0)	0 (0)
TS3	0 (**0.8**)	0 (**1**)	0 (**0.2**)	0 (0)	0 (**1**)	0 (**1**)	0 (**1**)
TS4	**1** (**0.2**)	**1** (0)	**1** (**0.8**)	**1** (**1**)	**0.5** (0)	**1** (0)	**1** (0)
I0	**1** (0)	**1** (**1**)	**1** (**1**)	**1** (0)	0 (0)	0 (0)	0 (0)
I1	0 (**1**)	0 (0)	0 (0)	0 (**1**)	**0.5** (**1**)	**1** (**1**)	**1** (**1**)
I2	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)
I3	0 (0)	0 (0)	0 (0)	0 (0)	**0.5** (0)	0 (0)	0 (0)

Table S16. Control degree of TSs and Is obtained with **ΔG** and **ΔE+ZPE**, shown in parenthesis, for **HCOOH formation**.

X_{TOF}	H	Mes'	Mes	FMes	CF_3	PFtB	C_6F_5
TS1	0 (**1**)	0 (**1**)	0 (**1**)	0 (**1**)	0 (**1**)	0 (**1**)	0 (**1**)
TS2	**1** (0)	**1** (0)	**1** (0)	**1** (0)	**1** (0)	**1** (0)	**1** (0)
I0	**1** (0)	**1** (0)	**1** (**0.2**)	**1** (0)	0 (0)	0 (0)	0 (0)
I1	0 (**1**)	0 (**1**)	0 (**0.8**)	0 (**1**)	**1** (**1**)	**1** (**1**)	**1** (**1**)

6. Cartesian Coordinates

The electronic energy reported was computed at (SMD)/M06-2X/6-311+G(d,p)//M06-2X/6-31G(d,p) level of theory (SMD: benzene).

1. FLPs

H

E(RM062X) = -391.578661426

6	-0.290715000	-0.083299000	-0.017452000
6	1.106334000	0.190130000	0.079543000
5	2.206512000	-0.863825000	-0.088913000
6	-0.164470000	-1.759020000	-1.831232000
1	0.699978000	-1.158698000	-2.112990000
1	0.152273000	-2.802638000	-1.738361000
1	-0.904452000	-1.689066000	-2.641534000
6	-2.125679000	-1.649155000	-0.418989000
1	-2.227508000	-2.704789000	-0.683049000
1	-2.426509000	-1.531865000	0.623873000
1	-2.814458000	-1.070565000	-1.055820000
7	-0.741107000	-1.264442000	-0.589377000
1	1.963295000	-2.028696000	-0.170232000
1	3.349081000	-0.513807000	-0.069144000
6	1.501041000	1.441101000	0.594599000
1	2.565975000	1.652596000	0.645369000
6	0.594917000	2.371975000	1.077399000
1	0.929555000	3.318553000	1.486508000
6	-1.206227000	0.854469000	0.495917000
1	-2.271862000	0.667792000	0.440212000
6	-0.762308000	2.053652000	1.035778000
1	-1.495978000	2.762762000	1.408813000

Mes'

E(RM062X) = -1089.48819144

7	-2.212893000	-0.906747000	0.421029000
6	-2.462191000	0.062083000	-0.618383000
6	-1.354201000	0.786409000	-1.072557000
5	0.025310000	0.493424000	-0.357948000
6	1.125180000	-0.285912000	-1.154073000
6	0.682462000	-1.215702000	-2.112112000
6	2.518651000	-0.156859000	-0.960200000
6	1.537732000	-2.042114000	-2.833096000
6	3.377384000	-0.965532000	-1.706319000
6	2.919594000	-1.911784000	-2.622034000
6	0.222429000	0.914024000	1.142213000
6	0.711596000	-0.069420000	2.015746000
6	-0.162825000	2.151071000	1.690402000
6	0.807462000	0.115893000	3.392145000
6	-0.038469000	2.349213000	3.067045000
6	0.426654000	1.357081000	3.928489000
6	3.135115000	0.842186000	-0.006854000
1	2.560527000	1.768961000	0.046423000
1	3.184636000	0.444947000	1.011620000
1	4.152748000	1.085228000	-0.323418000
6	3.892363000	-2.767892000	-3.388259000
1	3.715481000	-3.832552000	-3.200818000
1	3.790402000	-2.615076000	-4.468168000
1	4.923164000	-2.540946000	-3.109325000
6	-0.708588000	3.267712000	0.831511000
1	-1.730820000	3.051069000	0.503675000
1	-0.720574000	4.211088000	1.382808000
1	-0.110315000	3.413665000	-0.073050000
6	0.527260000	1.613073000	5.409058000
1	-0.076569000	0.898288000	5.978725000
1	1.558967000	1.508535000	5.762378000
1	0.185179000	2.619453000	5.658745000
6	-2.638085000	-2.253154000	0.070744000
1	-2.265498000	-2.949992000	0.827593000
1	-3.734064000	-2.368972000	0.014570000
1	-2.210460000	-2.532021000	-0.895450000
6	-2.740407000	-0.493055000	1.715016000
1	-3.843749000	-0.478959000	1.739666000
1	-2.383626000	-1.186511000	2.483249000
1	-2.367215000	0.504432000	1.959696000
6	-1.536028000	1.685108000	-2.129718000
1	-0.681862000	2.232592000	-2.522001000
6	-2.795807000	1.892337000	-2.685092000
1	-2.921782000	2.599751000	-3.498770000
6	-3.726733000	0.258022000	-1.175758000
1	-4.575314000	-0.314935000	-0.810552000
6	-3.893495000	1.180168000	-2.205044000
1	-4.875702000	1.334902000	-2.640674000
1	4.451599000	-0.852739000	-1.571036000
1	-0.321465000	3.312929000	3.486810000

1	1.014532000	-1.028818000	1.597304000
6	1.317506000	-0.983750000	4.286853000
1	0.567189000	-1.276829000	5.029667000
1	1.578695000	-1.869990000	3.704858000
1	2.207915000	-0.669581000	4.842441000
1	-0.387661000	-1.295098000	-2.296035000
6	0.999980000	-3.038312000	-3.826673000
1	-0.090370000	-2.995636000	-3.868833000
1	1.384190000	-2.848129000	-4.834822000
1	1.287948000	-4.062274000	-3.564112000

Mes

E(RM062X) = -1089.48409909

7	-2.536150000	-0.714279000	0.586565000
6	-2.507248000	0.209577000	-0.520533000
6	-1.253348000	0.625468000	-0.996072000
5	0.085593000	0.187570000	-0.284230000
6	1.217786000	-0.484628000	-1.148331000
6	0.901320000	-1.523198000	-2.057227000
6	2.568820000	-0.075487000	-1.045684000
6	1.902706000	-2.107714000	-2.829802000
6	3.537732000	-0.662182000	-1.860389000
6	3.226372000	-1.678670000	-2.759496000
6	0.280719000	0.515000000	1.244850000
6	0.518016000	-0.528187000	2.163516000
6	0.178591000	1.833650000	1.729773000
6	0.652808000	-0.241112000	3.521195000
6	0.344434000	2.089728000	3.091597000
6	0.582177000	1.064756000	4.004881000
6	-3.401728000	-1.865504000	0.364852000
1	-3.194221000	-2.614963000	1.135416000
1	-4.476749000	-1.623384000	0.416542000
1	-3.194445000	-2.304213000	-0.614050000
6	-2.865150000	-0.066543000	1.853877000
1	-3.921361000	0.251306000	1.894834000
1	-2.679955000	-0.770258000	2.672155000
1	-2.226142000	0.804427000	2.006257000
6	-1.213357000	1.447667000	-2.129460000
1	-0.246842000	1.740619000	-2.534834000
6	-2.379972000	1.886925000	-2.749628000
1	-2.325973000	2.528606000	-3.623316000
6	-3.678037000	0.636375000	-1.148317000
1	-4.642385000	0.299954000	-0.777353000
6	-3.615850000	1.479651000	-2.255165000
1	-4.531709000	1.805835000	-2.738199000
1	4.568812000	-0.323779000	-1.781199000
1	0.277030000	3.115331000	3.449798000
1	1.643598000	-2.921152000	-3.504627000
1	0.819523000	-1.058340000	4.220619000
6	0.780959000	1.359328000	5.469356000
1	0.392205000	0.549750000	6.092298000
1	1.844734000	1.471965000	5.704065000
1	0.279598000	2.286018000	5.759015000
6	0.566382000	-1.964902000	1.701435000
1	1.369184000	-2.126213000	0.975713000
1	0.722450000	-2.643151000	2.543675000
1	-0.378935000	-2.232086000	1.214047000
6	-0.136585000	2.991775000	0.809191000
1	0.439237000	2.955669000	-0.121298000
1	-1.193579000	2.986450000	0.520822000
1	0.077516000	3.945139000	1.298103000
6	3.025719000	0.989221000	-0.072528000
1	2.415176000	1.894103000	-0.127940000
1	2.968398000	0.632705000	0.960044000
1	4.060501000	1.271360000	-0.280070000
6	4.285676000	-2.286274000	-3.641291000
1	4.068857000	-3.335783000	-3.854927000
1	4.340739000	-1.759839000	-4.600061000
1	5.272028000	-2.226096000	-3.175110000
6	-0.502112000	-2.074252000	-2.185064000
1	-1.141277000	-1.411289000	-2.776547000
1	-0.482300000	-3.052407000	-2.671730000
1	-0.976634000	-2.190580000	-1.206059000

FMes

E(RM062X) = -2875.93166574

7	-3.106294000	-0.410449000	0.795755000
6	-3.070149000	0.307887000	-0.452673000
6	-1.834506000	0.451719000	-1.107109000
5	-0.493729000	0.042528000	-0.402341000
6	0.684621000	-0.610652000	-1.279540000
6	0.384609000	-1.433262000	-2.390571000
6	2.059347000	-0.299636000	-1.120849000
6	1.338445000	-1.776001000	-3.347393000
6	3.011404000	-0.629232000	-2.080635000
6	2.639802000	-1.327669000	-3.218508000
6	-0.362538000	0.586282000	1.094223000
6	-0.417255000	-0.239442000	2.222310000
6	-0.309780000	1.964995000	1.347983000
6	-0.409871000	0.256546000	3.518084000
6	-0.290413000	2.487034000	2.638534000
6	-0.344312000	1.628355000	3.725354000
6	2.622070000	0.310442000	0.150981000
6	3.652753000	-1.612848000	-4.294126000
6	-0.320847000	2.964481000	0.219126000
6	-0.396101000	2.170559000	5.125620000
6	-3.864076000	-1.655820000	0.702439000
1	-3.719576000	-2.223978000	1.624799000
1	-4.944646000	-1.486852000	0.562357000
1	-3.492598000	-2.248356000	-0.133449000
6	-3.578866000	0.409517000	1.905202000
1	-4.650606000	0.657886000	1.835792000
1	-3.412756000	-0.136844000	2.839532000
1	-3.008888000	1.342538000	1.940581000
6	-1.814637000	1.096949000	-2.352715000
1	-0.870684000	1.210804000	-2.879079000
6	-2.972325000	1.620291000	-2.915214000
1	-2.929951000	2.128938000	-3.872449000
6	-4.234249000	0.819991000	-1.023767000
1	-5.183536000	0.692860000	-0.510400000
6	-4.185221000	1.482665000	-2.246438000
1	-5.095621000	1.883064000	-2.681395000
1	4.049791000	-0.363152000	-1.930572000
1	-0.226531000	3.558715000	2.790702000
6	-0.958232000	-2.107610000	-2.627410000
1	1.064945000	-2.413194000	-4.180552000
1	-0.453826000	-0.424043000	4.363069000
6	-0.501248000	-1.732485000	2.085917000
9	-1.668563000	-2.268126000	-1.507169000
9	-0.757887000	-3.339796000	-3.127730000
9	-1.715401000	-1.460267000	-3.518361000
9	3.686082000	-0.624377000	-5.197351000
9	4.885529000	-1.730434000	-3.786675000
9	3.365453000	-2.743370000	-4.950037000
9	2.231696000	-0.393844000	1.223367000
9	2.268005000	1.586223000	0.344961000
9	3.962215000	0.290531000	0.148875000
9	-0.638018000	-2.122071000	0.808474000
9	0.594306000	-2.331797000	2.569584000
9	-1.545913000	-2.223851000	2.771818000
9	0.129760000	3.399004000	5.201012000
9	0.270048000	1.382192000	5.979328000
9	-1.659544000	2.249407000	5.568864000

9	0.356576000	4.074006000	0.536390000
9	0.234883000	2.470418000	-0.904620000
9	-1.569506000	3.336981000	-0.089745000

CF_3

E(RM062X) = -1065.69168964

7	-1.397212000	-1.418218000	1.207968000
6	-1.810352000	-0.209943000	0.654858000
6	-0.954528000	0.428140000	-0.283084000
5	0.532116000	0.140634000	-0.347113000
6	-2.021145000	-1.849989000	2.442145000
1	-3.032198000	-2.260838000	2.289920000
1	-1.401162000	-2.631815000	2.887553000
1	-2.073901000	-1.014730000	3.142731000
6	-1.103193000	-2.536012000	0.315836000
1	-2.005617000	-3.140944000	0.137974000
1	-0.741314000	-2.172182000	-0.645871000
1	-0.330988000	-3.169013000	0.757136000
6	1.423855000	-0.360921000	0.900599000
9	2.641836000	0.221660000	0.860702000
9	0.912232000	-0.064527000	2.105158000
9	1.633278000	-1.695202000	0.864739000
6	1.414215000	0.526210000	-1.635485000
9	1.911938000	1.773358000	-1.498414000
9	2.454114000	-0.308770000	-1.809112000
9	0.717389000	0.513888000	-2.790113000
6	-1.421490000	1.570714000	-0.966637000
1	-0.786209000	2.036978000	-1.713370000
6	-2.640639000	2.147228000	-0.647404000
1	-2.976272000	3.044381000	-1.154577000
6	-3.027751000	0.396280000	0.993045000
1	-3.683485000	-0.060648000	1.724994000
6	-3.423570000	1.563157000	0.349793000
1	-4.378742000	2.008549000	0.611951000

PFtB

E(RM062X) = -2492.44015028

7	-2.018374000	-2.076375000	0.440249000
6	-2.646376000	-0.777594000	0.401910000
6	-1.828307000	0.344185000	0.208745000
5	-0.267860000	0.195534000	0.065789000
6	0.679408000	0.615699000	1.400340000
6	0.293707000	-0.133604000	-1.477084000
6	-0.232114000	1.038106000	2.594073000
9	-1.043630000	2.045378000	2.285076000
9	-0.984101000	0.005309000	2.991039000
9	0.477617000	1.439648000	3.650145000
6	1.713778000	1.772248000	1.270301000
9	2.567625000	1.741809000	2.299773000
9	2.447594000	1.726217000	0.167865000
9	1.089934000	2.954053000	1.291203000
6	1.443964000	-0.655236000	1.846707000
9	1.681634000	-0.699612000	3.155360000
9	0.715532000	-1.739650000	1.539922000
9	2.616829000	-0.751836000	1.223610000
6	1.659310000	-0.870588000	-1.615654000
9	2.698817000	-0.127249000	-1.262402000
9	1.649789000	-1.965148000	-0.851729000
9	1.887128000	-1.264352000	-2.871905000
6	0.349487000	1.290312000	-2.101436000
9	0.361904000	2.215674000	-1.110095000
9	1.417919000	1.490172000	-2.859101000
9	-0.735550000	1.565771000	-2.821898000
6	-0.670887000	-0.964700000	-2.384232000
9	-0.369445000	-0.780776000	-3.676869000
9	-0.543530000	-2.266803000	-2.127835000
9	-1.953380000	-0.636996000	-2.256627000
6	-2.673877000	-3.043964000	-0.446763000
1	-2.005091000	-3.897782000	-0.583949000
1	-3.621478000	-3.417992000	-0.028535000
1	-2.872150000	-2.596144000	-1.418454000
6	-1.978981000	-2.656079000	1.786797000
1	-2.990073000	-2.897615000	2.153070000
1	-1.395823000	-3.580392000	1.750105000
1	-1.505185000	-1.978161000	2.488356000
6	-2.435723000	1.598868000	0.055332000
1	-1.822962000	2.479521000	-0.108708000
6	-3.817358000	1.736810000	0.109382000
1	-4.266430000	2.715070000	-0.024266000
6	-4.030693000	-0.630969000	0.486352000
1	-4.652055000	-1.506759000	0.648331000
6	-4.616537000	0.621246000	0.339813000
1	-5.695275000	0.724819000	0.397178000

C_6F_5

E(RM062X) = -1845.99811827

7	-2.686534000	-1.771928000	-0.229288000
6	-3.039839000	-0.537012000	0.319116000
6	-2.015164000	0.365624000	0.704674000
5	-0.529645000	0.204386000	0.306222000
6	-1.758326000	-2.635451000	0.484143000
1	-1.215446000	-2.068841000	1.243395000
1	-2.294814000	-3.448168000	0.996212000
1	-1.033154000	-3.081666000	-0.206726000
6	-3.677163000	-2.505033000	-0.986491000
1	-3.165675000	-3.269175000	-1.579128000
1	-4.422374000	-3.011677000	-0.351955000
1	-4.191439000	-1.829352000	-1.673232000
6	0.577724000	0.775360000	1.272806000
6	0.490532000	0.598145000	2.654584000
6	1.699322000	1.468619000	0.816428000
6	1.447092000	1.083039000	3.536738000
6	2.666086000	1.981650000	1.666938000
6	2.535593000	1.784557000	3.036696000
6	-0.081286000	-0.448648000	-1.057499000
6	1.131481000	-1.129143000	-1.186175000
6	-0.870903000	-0.405499000	-2.211451000
6	1.540541000	-1.742858000	-2.362361000
6	-0.490559000	-0.998710000	-3.405855000
6	0.721824000	-1.673366000	-3.479913000
9	1.333445000	0.879975000	4.846272000
9	-0.520058000	-0.095882000	3.183997000
9	3.454634000	2.261895000	3.864575000
9	3.710994000	2.652893000	1.191668000
9	1.869430000	1.673188000	-0.492264000
9	1.957154000	-1.244273000	-0.140924000
9	2.700250000	-2.392015000	-2.425190000
9	1.093476000	-2.248365000	-4.615529000
9	-1.273108000	-0.928407000	-4.480283000
9	-2.039357000	0.233296000	-2.217460000
6	-2.389939000	1.564999000	1.333396000
1	-1.610698000	2.251752000	1.654414000
6	-3.720581000	1.927868000	1.495970000
1	-3.982732000	2.872741000	1.958325000
6	-4.381090000	-0.164759000	0.472738000
1	-5.172451000	-0.842703000	0.174655000
6	-4.710459000	1.059122000	1.045365000
1	-5.757475000	1.321973000	1.163092000

2. FLP + H_2 (TS)

H

E(RM062X) = -392.745291061

6	-1.318005000	1.682418000	0.632916000
6	0.028507000	1.849390000	0.984705000
5	1.042121000	0.627009000	0.792090000
6	-1.610450000	0.308732000	-1.342517000
1	-0.648971000	0.695635000	-1.683861000
1	-1.716456000	-0.729914000	-1.667479000
1	-2.418558000	0.909476000	-1.779473000
6	-2.875302000	-0.219419000	0.667456000
1	-2.918697000	-1.275961000	0.390627000
1	-2.863030000	-0.132200000	1.754943000
1	-3.774220000	0.276500000	0.279224000
7	-1.649003000	0.363877000	0.124552000
1	-0.371522000	-0.238095000	0.622354000
1	0.385189000	-0.551829000	0.994013000
1	1.477948000	0.480224000	-0.321444000
1	1.836433000	0.459079000	1.676329000
6	0.392207000	3.104893000	1.484787000
1	1.422926000	3.273859000	1.783503000
6	-0.536919000	4.133505000	1.616004000
1	-0.225759000	5.097320000	2.007091000
6	-2.267397000	2.691482000	0.764979000
1	-3.303242000	2.520061000	0.484693000
6	-1.868574000	3.929596000	1.258825000
1	-2.594024000	4.729454000	1.366083000

Mes'

E(RM062X) = -1090.64428135

7	-0.981831000	0.950348000	0.765081000
6	-1.016301000	1.884850000	-0.346268000
6	0.228415000	2.348258000	-0.793370000
5	1.585089000	1.864702000	-0.048770000
6	2.804535000	1.498114000	-1.041973000
6	2.471070000	1.015382000	-2.319462000
6	4.180380000	1.578526000	-0.734309000
6	3.402531000	0.638116000	-3.282487000
6	5.117532000	1.211889000	-1.706359000
6	4.764785000	0.748655000	-2.970047000
6	1.826979000	2.599330000	1.368731000
6	1.752138000	1.902129000	2.581901000
6	2.105597000	3.977319000	1.444201000
6	1.925381000	2.496183000	3.831478000
6	2.285712000	4.578372000	2.691462000
6	2.196379000	3.870656000	3.888469000
6	4.715554000	2.032881000	0.604822000
1	4.508070000	3.090211000	0.794067000
1	4.267885000	1.477417000	1.432144000
1	5.798565000	1.890767000	0.642750000
6	5.819399000	0.366660000	-3.974916000
1	5.722918000	-0.682268000	-4.276467000
1	5.737294000	0.967228000	-4.887649000
1	6.822002000	0.509562000	-3.566324000
6	2.243712000	4.816836000	0.197606000
1	1.264646000	5.073543000	-0.220263000
1	2.773359000	5.748977000	0.410726000
1	2.797444000	4.278992000	-0.580341000
6	2.395346000	4.562259000	5.211776000
1	1.508377000	4.472456000	5.848853000
1	3.231659000	4.126595000	5.769523000
1	2.602040000	5.625341000	5.071536000
6	-1.675522000	-0.311732000	0.498048000
1	-1.475218000	-1.005526000	1.318787000
1	-2.760946000	-0.176727000	0.411776000
1	-1.295580000	-0.737780000	-0.432811000
6	-1.418611000	1.562366000	2.027353000
1	-2.500356000	1.753393000	2.011536000
1	-1.184005000	0.888802000	2.856645000
1	-0.882423000	2.500202000	2.173234000
6	0.206159000	3.228457000	-1.884688000
1	1.150826000	3.583666000	-2.288710000
6	-0.985780000	3.638405000	-2.473812000
1	-0.965306000	4.325019000	-3.314439000
6	-2.221428000	2.270746000	-0.929880000
1	-3.164199000	1.884219000	-0.551330000
6	-2.205585000	3.162202000	-1.995845000
1	-3.136908000	3.478416000	-2.454265000
1	6.175404000	1.285889000	-1.460182000
1	2.509897000	5.643276000	2.731374000
1	1.553654000	0.829365000	2.561654000
6	1.825007000	1.679379000	5.093675000
1	1.033909000	2.053907000	5.753173000
1	1.607584000	0.632913000	4.866879000
1	2.757022000	1.711148000	5.668668000
1	1.417832000	0.924765000	-2.579782000
6	2.960520000	0.126321000	-4.628901000
1	1.870904000	0.110438000	-4.702149000
1	3.343585000	0.752445000	-5.442532000
1	3.326491000	-0.890116000	-4.812722000
1	1.325718000	0.535414000	0.373596000
1	0.490443000	0.696083000	0.624829000

Mes

E(RM062X) = -1090.63691784

7	-1.315662000	1.541078000	0.658878000
6	-1.045071000	2.418537000	-0.455018000
6	0.290383000	2.588398000	-0.860711000
5	1.540220000	1.954730000	-0.086030000
6	2.719964000	1.412438000	-1.034988000
6	2.483996000	0.417228000	-2.016464000
6	4.020772000	1.969724000	-0.970575000
6	3.514144000	-0.008017000	-2.856892000
6	5.019912000	1.526968000	-1.839804000
6	4.794480000	0.529338000	-2.782530000
6	1.832199000	2.415265000	1.426978000
6	2.362383000	1.505738000	2.371425000
6	1.608099000	3.746127000	1.859484000
6	2.601330000	1.906017000	3.688833000
6	1.869806000	4.111020000	3.180729000
6	2.351542000	3.202953000	4.120230000
6	-2.329770000	0.532405000	0.373880000
1	-2.329225000	-0.206162000	1.181026000
1	-3.347232000	0.946877000	0.296568000
1	-2.087390000	0.026874000	-0.564142000
6	-1.608563000	2.255459000	1.899520000
1	-2.570192000	2.792024000	1.846654000
1	-1.655640000	1.536526000	2.722874000
1	-0.811160000	2.967951000	2.113687000
6	0.522848000	3.380394000	-1.994106000
1	1.545173000	3.493145000	-2.349005000
6	-0.510450000	4.023158000	-2.667502000
1	-0.294941000	4.639082000	-3.534895000
6	-2.088844000	3.049385000	-1.135495000
1	-3.113299000	2.904372000	-0.802979000
6	-1.823359000	3.862709000	-2.232031000
1	-2.638519000	4.357878000	-2.750220000
1	6.006562000	1.982025000	-1.778645000
1	1.700636000	5.142686000	3.483519000
1	1.046385000	0.380133000	0.219500000
1	0.378156000	0.691257000	0.468583000
1	3.304577000	-0.776789000	-3.598187000
1	3.008888000	1.182514000	4.392480000
6	2.589581000	3.615119000	5.549640000
1	1.662195000	3.566506000	6.130160000
1	3.317408000	2.960233000	6.034635000

1	2.959109000	4.642120000	5.609187000
6	2.708995000	0.074143000	2.023382000
1	3.422707000	-0.326402000	2.746796000
1	1.824553000	-0.573288000	2.050163000
1	3.152101000	-0.012307000	1.028099000
6	1.115402000	4.846542000	0.941489000
1	1.665103000	4.877903000	-0.002873000
1	0.059107000	4.726705000	0.678778000
1	1.232648000	5.817168000	1.429143000
6	4.403674000	3.067735000	-0.000762000
1	3.681843000	3.888044000	0.001602000
1	4.464554000	2.699970000	1.027551000
1	5.378052000	3.480750000	-0.272383000
6	5.900914000	0.040572000	-3.680703000
1	6.457549000	-0.774260000	-3.205705000
1	5.505480000	-0.338393000	-4.626340000
1	6.613304000	0.839263000	-3.901910000
6	1.141174000	-0.258622000	-2.194813000
1	1.101980000	-0.766850000	-3.160725000
1	0.968607000	-1.018785000	-1.423072000
1	0.311591000	0.450276000	-2.150673000

FMes

E(RM062X) = -2877.07532261

7	-1.056556000	1.799905000	0.979900000
6	-0.856277000	2.454000000	-0.289459000
6	0.430308000	2.457036000	-0.856333000
5	1.695323000	1.874324000	-0.095040000
6	2.860138000	1.250518000	-1.032914000
6	2.566760000	0.362664000	-2.106433000
6	4.202006000	1.704040000	-0.984535000
6	3.487737000	0.086395000	-3.112001000
6	5.115302000	1.440326000	-2.006814000
6	4.743127000	0.670854000	-3.090917000
6	1.898982000	2.385638000	1.425144000
6	2.120231000	1.545207000	2.535863000
6	1.770908000	3.759159000	1.726519000
6	2.089343000	2.015983000	3.845353000
6	1.765868000	4.240864000	3.033194000
6	1.886610000	3.362599000	4.095991000
6	4.808622000	2.415806000	0.217394000
6	5.691518000	0.446380000	-4.236259000
6	1.619812000	4.845777000	0.677059000
6	1.780302000	3.863561000	5.508622000
6	-1.946800000	0.645436000	0.871896000
1	-1.910296000	0.081977000	1.809465000
1	-2.993184000	0.928579000	0.675981000
1	-1.606468000	-0.002732000	0.060300000
6	-1.495522000	2.705190000	2.037196000
1	-2.546077000	3.017148000	1.917879000
1	-1.394238000	2.202800000	3.004596000
1	-0.871516000	3.599234000	2.036511000
6	0.576493000	3.031337000	-2.128591000
1	1.557951000	3.043374000	-2.595438000
6	-0.491265000	3.615667000	-2.796429000
1	-0.340389000	4.066398000	-3.771758000
6	-1.934546000	3.025619000	-0.965993000
1	-2.920783000	3.004739000	-0.509774000
6	-1.754431000	3.616718000	-2.210228000
1	-2.596570000	4.069052000	-2.724261000
1	6.125132000	1.823029000	-1.944982000
1	1.675532000	5.305148000	3.217775000
1	1.031796000	0.083767000	0.291153000
1	0.520228000	0.521718000	0.625703000
6	1.333235000	-0.533905000	-2.153299000
1	3.231450000	-0.597736000	-3.910558000
1	2.253690000	1.331575000	4.669994000
6	2.403234000	0.058051000	2.443343000
9	0.158999000	0.075320000	-1.980331000
9	1.434778000	-1.472850000	-1.193481000
9	1.246547000	-1.187159000	-3.320565000
9	5.446020000	1.298756000	-5.240602000
9	6.964800000	0.621970000	-3.864503000
9	5.572100000	-0.791998000	-4.731515000
9	4.653686000	1.690247000	1.333693000
9	4.301582000	3.630257000	0.449763000
9	6.129663000	2.588927000	0.062802000
9	2.933890000	-0.326691000	1.275005000
9	3.270202000	-0.312083000	3.396570000
9	1.288149000	-0.666306000	2.637581000
9	2.211938000	5.126135000	5.616767000
9	2.492816000	3.108915000	6.354218000
9	0.508384000	3.842016000	5.934220000
9	2.179636000	5.989177000	1.102476000
9	2.201349000	4.551776000	-0.491950000
9	0.329793000	5.122452000	0.430491000

CF_3

E(RM062X) = -1066.85648130

7	-0.659407000	0.079811000	0.399577000
6	-1.116608000	1.375647000	-0.032809000
6	-0.213564000	2.162405000	-0.765155000
5	1.268678000	1.722817000	-0.911323000
1	1.298286000	0.091221000	-1.885457000
1	0.975758000	-0.091931000	-1.228216000
6	-0.786065000	-0.136964000	1.839085000
1	-1.833624000	-0.249409000	2.161787000
1	-0.247011000	-1.051394000	2.102403000
1	-0.333734000	0.697074000	2.373351000
6	-1.320620000	-0.992015000	-0.344194000
1	-2.394854000	-1.068913000	-0.111208000
1	-1.219519000	-0.817613000	-1.418935000
1	-0.844657000	-1.945183000	-0.095782000
6	2.165052000	1.335516000	0.383463000
9	3.338334000	2.002507000	0.340557000
9	1.570785000	1.705086000	1.536001000
9	2.462695000	0.029654000	0.498357000
6	2.123670000	2.260998000	-2.163655000
9	2.471373000	3.546334000	-1.941439000
9	3.256128000	1.568667000	-2.382016000
9	1.430261000	2.236668000	-3.320183000
6	-0.653040000	3.389558000	-1.282551000
1	0.029608000	4.003357000	-1.862436000
6	-1.946057000	3.840921000	-1.040001000
1	-2.269924000	4.798697000	-1.433025000
6	-2.416355000	1.820453000	0.197770000
1	-3.109850000	1.200065000	0.758730000
6	-2.824523000	3.057073000	-0.296132000
1	-3.835977000	3.404215000	-0.109572000

PFtB

E(RM062X) = -2493.59669882

7	-0.871925000	0.091744000	0.358858000
6	-1.251346000	1.408798000	-0.082442000
6	-0.268302000	2.340284000	-0.472564000
5	1.294552000	2.057926000	-0.576343000
6	2.242398000	2.297637000	0.825793000
6	1.836485000	1.917168000	-2.176929000
6	1.373142000	2.043077000	2.104456000
9	0.179970000	2.633689000	2.052768000
9	1.195040000	0.725940000	2.245838000
9	1.937486000	2.488326000	3.227368000
6	2.666146000	3.794093000	0.849805000
9	3.312391000	4.124668000	1.965226000

9	3.472614000	4.092952000	-0.164590000
9	1.580354000	4.573630000	0.762341000
6	3.552410000	1.467653000	1.060510000
9	4.005100000	1.628941000	2.308501000
9	3.358570000	0.164290000	0.893058000
9	4.539048000	1.859171000	0.258106000
6	3.311496000	1.498294000	-2.382951000
9	4.126653000	2.513254000	-2.099761000
9	3.616738000	0.457660000	-1.605387000
9	3.567250000	1.121803000	-3.637713000
6	1.659393000	3.296525000	-2.886549000
9	1.926414000	4.308917000	-2.050808000
9	2.472628000	3.425677000	-3.931769000
9	0.412532000	3.460916000	-3.328278000
6	0.993652000	0.923256000	-3.039043000
9	1.163779000	1.166473000	-4.342046000
9	1.373026000	-0.338863000	-2.818857000
9	-0.313116000	1.004720000	-2.805199000
6	-1.241582000	-0.967658000	-0.578450000
1	-0.864501000	-1.919429000	-0.192112000
1	-2.333223000	-1.053518000	-0.703101000
1	-0.791150000	-0.793553000	-1.553631000
6	-1.398212000	-0.227728000	1.686885000
1	-2.469298000	-0.484491000	1.668545000
1	-0.849802000	-1.087229000	2.083636000
1	-1.252777000	0.617663000	2.358294000
1	1.202300000	-0.464719000	-0.127104000
1	1.763127000	-0.628360000	-0.586919000
6	-0.710214000	3.638864000	-0.785382000
1	-0.000161000	4.411346000	-1.044552000
6	-2.054017000	3.993028000	-0.745999000
1	-2.341935000	5.011311000	-0.984466000
6	-2.600018000	1.764036000	-0.076484000
1	-3.334291000	1.017258000	0.211968000
6	-3.011912000	3.048127000	-0.406731000
1	-4.065137000	3.308202000	-0.386827000

C_6F_5

E(RM062X) = -1847.15350399

7	-1.047683000	0.142926000	-0.385054000
6	-1.410114000	1.508680000	-0.090718000
6	-0.390058000	2.470897000	-0.071350000
5	1.119422000	2.142662000	-0.415984000
6	-1.409908000	-0.784196000	0.684044000
1	-0.995813000	-0.423523000	1.629208000
1	-2.497926000	-0.903606000	0.799779000
1	-0.981144000	-1.766027000	0.462788000
6	-1.552341000	-0.305526000	-1.681719000
1	-1.068707000	-1.248535000	-1.952759000
1	-2.642569000	-0.464146000	-1.669443000
1	-1.326225000	0.446110000	-2.438781000
6	2.203239000	2.831804000	0.531081000
6	2.062700000	2.764407000	1.917910000
6	3.291458000	3.568201000	0.069116000
6	2.937920000	3.379608000	2.800687000
6	4.183202000	4.208584000	0.920830000
6	4.003843000	4.111864000	2.293394000
6	1.537004000	1.746800000	-1.901004000
6	2.752822000	1.111789000	-2.153649000
6	0.748849000	2.001477000	-3.019252000
6	3.170358000	0.736760000	-3.419477000
6	1.131551000	1.643424000	-4.307942000
6	2.348552000	1.010470000	-4.507148000
9	2.769147000	3.275909000	4.116243000
9	1.064367000	2.049016000	2.446792000
9	4.849253000	4.715115000	3.119360000
9	5.202136000	4.911513000	0.433673000
9	3.515205000	3.704113000	-1.241363000
9	3.567283000	0.828823000	-1.129906000
9	4.336662000	0.124930000	-3.606125000
9	2.727330000	0.661300000	-5.730042000
9	0.338863000	1.901470000	-5.345505000
9	-0.441047000	2.599882000	-2.902334000
1	0.804466000	0.414027000	0.048895000
1	1.494442000	0.631997000	0.338306000
6	-0.742198000	3.789750000	0.242930000
1	0.032806000	4.551378000	0.281928000
6	-2.060523000	4.148693000	0.503655000
1	-2.306909000	5.179851000	0.734743000
6	-2.729879000	1.858463000	0.191898000
1	-3.503321000	1.095089000	0.179793000
6	-3.058560000	3.179039000	0.479339000
1	-4.088884000	3.448186000	0.688413000

3. FLP-H^+/H^-

H

E(RM062X) = -392.764697108

6	-0.205282000	-0.053538000	-0.011453000
6	1.135874000	0.073633000	0.353941000
5	2.148000000	-1.178122000	0.150755000
6	-0.537392000	-1.415963000	-2.028751000
1	0.430850000	-1.038322000	-2.355745000
1	-0.678935000	-2.442156000	-2.372601000
1	-1.344041000	-0.776485000	-2.391243000
6	-1.756739000	-2.004405000	0.040123000
1	-1.825591000	-3.040888000	-0.292976000
1	-1.674486000	-1.960052000	1.125494000
1	-2.638857000	-1.454301000	-0.289182000
7	-0.541841000	-1.394381000	-0.543558000
1	0.315252000	-1.940427000	-0.212797000
1	1.559388000	-2.233370000	0.491508000
1	2.417116000	-1.288957000	-1.036834000
1	3.140763000	-1.080745000	0.828696000
6	1.477520000	1.340742000	0.852932000
1	2.503510000	1.508522000	1.167350000
6	0.548621000	2.371792000	0.955498000
1	0.854914000	3.337472000	1.346700000
6	-1.170409000	0.942457000	0.068726000
1	-2.198195000	0.773928000	-0.242458000
6	-0.777498000	2.181177000	0.562928000
1	-1.498902000	2.987152000	0.643033000

Mes'

E(RM062X) = -1090.66668076

7	-2.636562000	-0.706655000	1.014657000
6	-2.583826000	0.008015000	-0.288190000
6	-1.332039000	0.060630000	-0.903126000
5	-0.004313000	-0.584856000	-0.149249000
6	1.249054000	-0.761414000	-1.172311000
6	0.963960000	-1.417383000	-2.383440000
6	2.593856000	-0.388346000	-0.972947000
6	1.898259000	-1.683281000	-3.379690000
6	3.538997000	-0.649324000	-1.973985000
6	3.225392000	-1.278385000	-3.173262000
6	0.197344000	0.229863000	1.263887000
6	0.213931000	-0.478136000	2.477488000
6	0.244988000	1.637077000	1.364366000
6	0.249676000	0.121092000	3.739290000
6	0.278362000	2.246216000	2.621877000
6	0.269933000	1.520748000	3.813917000
6	3.097737000	0.261910000	0.297069000
1	2.714212000	1.278620000	0.425839000
1	2.796914000	-0.299260000	1.184872000

1	4.189637000	0.319710000	0.283181000
6	4.282341000	-1.532262000	-4.216355000
1	4.385436000	-2.601664000	-4.432982000
1	4.038231000	-1.040188000	-5.164848000
1	5.255412000	-1.161088000	-3.886575000
6	0.275112000	2.511457000	0.132704000
1	-0.734728000	2.727118000	-0.234908000
1	0.764824000	3.465802000	0.346794000
1	0.813181000	2.018840000	-0.682818000
6	0.307155000	2.222625000	5.146734000
1	-0.555478000	1.957067000	5.768387000
1	1.202366000	1.949970000	5.716556000
1	0.308684000	3.307286000	5.019124000
6	-3.481895000	-1.926996000	0.959822000
1	-3.402190000	-2.454589000	1.911396000
1	-4.516603000	-1.639436000	0.774287000
1	-3.112825000	-2.550225000	0.145746000
6	-2.972184000	0.184186000	2.159607000
1	-3.997675000	0.535221000	2.039098000
1	-2.865380000	-0.382767000	3.085618000
1	-2.268844000	1.018188000	2.153821000
6	-1.335616000	0.731020000	-2.138876000
1	-0.395945000	0.809161000	-2.679189000
6	-2.485076000	1.293526000	-2.683927000
1	-2.432600000	1.805729000	-3.639883000
6	-3.760294000	0.553296000	-0.791045000
1	-4.700296000	0.474248000	-0.250141000
6	-3.705500000	1.211130000	-2.012901000
1	-4.602433000	1.651196000	-2.434914000
1	4.572410000	-0.350911000	-1.802357000
1	0.318665000	3.333715000	2.676710000
1	0.206647000	-1.569307000	2.431806000
6	0.268944000	-0.715573000	4.992926000
1	-0.585254000	-0.493294000	5.643531000
1	0.244816000	-1.781053000	4.752871000
1	1.170895000	-0.527311000	5.585591000
1	-0.061857000	-1.745244000	-2.557364000
6	1.500117000	-2.393046000	-4.648224000
1	0.433343000	-2.628760000	-4.645236000
1	1.708032000	-1.782668000	-5.534603000
1	2.052059000	-3.331489000	-4.775200000
1	-0.356213000	-1.732151000	0.184242000
1	-1.658192000	-1.027647000	1.142883000

Mes

E(RM062X) = -1090.66061860

7	-2.660503000	-0.332677000	0.923207000
6	-2.508958000	0.412472000	-0.356091000
6	-1.245075000	0.353031000	-0.943983000
5	-0.029679000	-0.465865000	-0.194471000
6	1.226973000	-0.772324000	-1.186078000
6	1.007877000	-1.666319000	-2.267823000
6	2.527962000	-0.232174000	-1.069664000
6	2.017875000	-1.957974000	-3.184513000
6	3.522015000	-0.550300000	-2.003145000
6	3.289211000	-1.401285000	-3.075694000
6	0.238122000	0.177672000	1.305920000
6	0.539649000	-0.703736000	2.375249000
6	0.102289000	1.548953000	1.637025000
6	0.634290000	-0.243133000	3.691600000
6	0.208126000	1.981821000	2.963137000
6	0.458321000	1.100231000	4.011766000
6	-3.446997000	-1.580553000	0.736439000
1	-3.451465000	-2.141790000	1.672239000
1	-4.463964000	-1.315765000	0.445522000
1	-2.962746000	-2.156081000	-0.052853000
6	-3.137338000	0.495680000	2.061575000
1	-4.165150000	0.807525000	1.876323000
1	-3.081038000	-0.104073000	2.971267000
1	-2.475185000	1.357052000	2.148842000
6	-1.150402000	1.018647000	-2.176801000
1	-0.193926000	0.992826000	-2.694744000
6	-2.224994000	1.697829000	-2.740829000
1	-2.103904000	2.204767000	-3.693367000
6	-3.613585000	1.073843000	-0.881283000
1	-4.572923000	1.078196000	-0.369612000
6	-3.461161000	1.735943000	-2.093675000
1	-4.299426000	2.267178000	-2.530996000
1	4.512874000	-0.115527000	-1.882102000
1	0.108110000	3.044845000	3.180247000
1	-0.553285000	-1.560745000	0.038917000
1	-1.688324000	-0.618395000	1.145461000
1	1.809051000	-2.647168000	-4.001657000
1	0.868443000	-0.951243000	4.485324000
6	0.599467000	1.591257000	5.430066000
1	0.286566000	0.828230000	6.147734000
1	1.640971000	1.844152000	5.655037000
1	0.000452000	2.489432000	5.601711000
6	0.808151000	-2.170505000	2.116970000
1	1.297911000	-2.629477000	2.979610000
1	-0.112460000	-2.730359000	1.913965000
1	1.445039000	-2.299682000	1.237402000
6	-0.118884000	2.620990000	0.588430000
1	0.380899000	2.373334000	-0.349998000
1	-1.179589000	2.763900000	0.347126000
1	0.271358000	3.578573000	0.944300000
6	2.942708000	0.684057000	0.062150000
1	2.329478000	1.586322000	0.113890000
1	2.857414000	0.192522000	1.035379000
1	3.982331000	0.996087000	-0.068353000
6	4.362046000	-1.703447000	-4.090552000
1	4.352142000	-2.759336000	-4.375868000
1	4.218261000	-1.117995000	-5.005238000
1	5.354572000	-1.466177000	-3.699306000
6	-0.315443000	-2.375137000	-2.458066000
1	-0.300506000	-2.979128000	-3.368976000
1	-0.524707000	-3.039135000	-1.612195000
1	-1.153696000	-1.675868000	-2.529291000

FMes

E(RM062X) = -2877.12405481

7	-3.864848000	-0.238520000	-0.206200000
6	-3.330339000	0.617708000	-1.307529000
6	-1.948793000	0.821436000	-1.360964000
5	-0.883047000	-0.030160000	-0.430126000
6	0.430016000	-0.402199000	-1.378341000
6	0.432839000	-1.561335000	-2.195070000
6	1.631709000	0.339057000	-1.428590000
6	1.555486000	-2.002314000	-2.886815000
6	2.764223000	-0.090297000	-2.121867000
6	2.737100000	-1.279389000	-2.824155000
6	-0.368306000	0.457171000	1.084625000
6	0.522927000	-0.372062000	1.818260000
6	-0.688756000	1.666862000	1.752667000
6	1.113124000	0.022897000	3.019382000
6	-0.105143000	2.068471000	2.950478000
6	0.825291000	1.255489000	3.572573000
6	1.831026000	1.656585000	-0.711114000
6	3.967668000	-1.792925000	-3.512333000
6	-1.782159000	2.580780000	1.259003000
6	1.504346000	1.717918000	4.827968000
6	-4.109678000	-1.645638000	-0.651579000
1	-4.529665000	-2.205394000	0.185586000

1	-4.815691000	-1.610459000	-1.481315000
1	-3.168090000	-2.080047000	-0.973547000
6	-5.087603000	0.306648000	0.456655000
1	-5.949490000	0.089110000	-0.172687000
1	-5.205955000	-0.193356000	1.418308000
1	-4.974436000	1.377804000	0.591181000
6	-1.540420000	1.619509000	-2.443457000
1	-0.481838000	1.818745000	-2.565760000
6	-2.426678000	2.158234000	-3.367838000
1	-2.049109000	2.769324000	-4.181370000
6	-4.252642000	1.120487000	-2.218598000
1	-5.313822000	0.909463000	-2.124558000
6	-3.792259000	1.907284000	-3.265013000
1	-4.490786000	2.314019000	-3.987783000
1	3.664605000	0.512445000	-2.118187000
1	-0.384844000	3.009596000	3.407016000
1	-1.449512000	-1.077273000	-0.206833000
1	-3.100155000	-0.261510000	0.479938000
6	-0.816795000	-2.384696000	-2.424804000
1	1.509974000	-2.900954000	-3.489440000
1	1.801043000	-0.640634000	3.528138000
6	1.014525000	-1.740087000	1.367636000
9	-1.870134000	-1.616408000	-2.762457000
9	-1.204188000	-3.122244000	-1.368527000
9	-0.657395000	-3.255604000	-3.435779000
9	3.662658000	-2.437396000	-4.649026000
9	4.814488000	-0.800821000	-3.820949000
9	4.640400000	-2.660507000	-2.742227000
9	2.277249000	1.505339000	0.545546000
9	0.713879000	2.394594000	-0.655048000
9	2.746466000	2.413900000	-1.343145000
9	0.113434000	-2.468150000	0.706841000
9	2.108246000	-1.648632000	0.592997000
9	1.376121000	-2.485915000	2.431267000
9	1.973375000	0.689013000	5.546962000
9	0.664054000	2.412980000	5.611063000
9	2.543070000	2.522978000	4.563324000
9	-2.027703000	3.591924000	2.105694000
9	-1.586383000	3.131115000	0.065858000
9	-2.955670000	1.885118000	1.188903000

CF_3

E(RM062X) = -1066.91747888

7	-1.374304000	-1.727288000	0.926286000
6	-1.796792000	-0.396901000	0.412156000
6	-0.836920000	0.342700000	-0.274674000
5	0.656566000	-0.242975000	-0.543470000
1	0.592101000	-1.384801000	-0.973359000
1	-0.397800000	-1.840221000	0.612520000
6	-1.343587000	-1.765026000	2.417352000
1	-2.363821000	-1.671139000	2.788562000
1	-0.902769000	-2.710408000	2.734546000
1	-0.728455000	-0.932113000	2.753570000
6	-2.149850000	-2.849528000	0.331470000
1	-3.192787000	-2.761213000	0.633554000
1	-2.065784000	-2.776570000	-0.752303000
1	-1.733260000	-3.792783000	0.686415000
6	1.502497000	-0.312354000	0.851766000
9	2.829662000	-0.190304000	0.727771000
9	1.120037000	0.590210000	1.791293000
9	1.320528000	-1.537780000	1.495816000
6	1.459518000	0.637330000	-1.626031000
9	1.742785000	1.896678000	-1.186214000
9	2.643501000	0.102576000	-1.989038000
9	0.760897000	0.812018000	-2.778832000
6	-1.276075000	1.603050000	-0.714587000
1	-0.580357000	2.236415000	-1.253137000
6	-2.569717000	2.057388000	-0.483906000
1	-2.866431000	3.037491000	-0.843357000
6	-3.099627000	0.018178000	0.666169000
1	-3.800212000	-0.607314000	1.213207000
6	-3.489193000	1.268642000	0.206012000
1	-4.497765000	1.623242000	0.387753000

PFtB

E(RM062X) = -2493.68458741

7	-2.352373000	-2.102060000	0.909028000
6	-2.731899000	-0.711988000	0.531970000
6	-1.721712000	0.186885000	0.169460000
5	-0.141896000	-0.256639000	0.038254000
6	0.793387000	0.321021000	1.405574000
6	0.367530000	-0.103995000	-1.605238000
6	-0.117218000	0.175494000	2.649455000
9	-1.185357000	0.974138000	2.616679000
9	-0.581530000	-1.104616000	2.724699000
9	0.467040000	0.408092000	3.823507000
6	1.253197000	1.787180000	1.375593000
9	1.802493000	2.166709000	2.541999000
9	2.163651000	2.015118000	0.434437000
9	0.217484000	2.611127000	1.158349000
6	2.042438000	-0.558912000	1.690241000
9	2.566425000	-0.353391000	2.908900000
9	1.738481000	-1.863214000	1.630141000
9	3.032145000	-0.321341000	0.834253000
6	1.826757000	-0.553648000	-1.818324000
9	2.671301000	0.434374000	-1.519010000
9	2.119242000	-1.621603000	-1.069002000
9	2.086782000	-0.912349000	-3.085851000
6	0.207655000	1.276251000	-2.268511000
9	0.511399000	2.277728000	-1.437010000
9	0.980100000	1.423819000	-3.351782000
9	-1.058952000	1.471164000	-2.671954000
6	-0.480559000	-1.077120000	-2.454319000
9	-0.328998000	-0.890908000	-3.768968000
9	-0.146972000	-2.355720000	-2.192631000
9	-1.800183000	-0.981664000	-2.221872000
6	-2.661771000	-3.103124000	-0.154243000
1	-2.381772000	-4.092766000	0.209333000
1	-3.731333000	-3.061742000	-0.360599000
1	-2.096302000	-2.848825000	-1.046157000
6	-2.913642000	-2.529088000	2.224208000
1	-3.966321000	-2.777122000	2.093834000
1	-2.366231000	-3.410029000	2.560948000
1	-2.797047000	-1.714520000	2.933608000
1	-1.323682000	-2.054292000	0.991153000
1	-0.057397000	-1.459042000	0.168791000
6	-2.189474000	1.484287000	-0.106005000
1	-1.472336000	2.252693000	-0.360757000
6	-3.533544000	1.830031000	-0.060504000
1	-3.831294000	2.848519000	-0.286959000
6	-4.089326000	-0.408272000	0.573859000
1	-4.824418000	-1.160558000	0.845407000
6	-4.497342000	0.881164000	0.268815000
1	-5.549829000	1.140520000	0.297046000

C_6F_5

E(RM062X) = -1847.19721785

7	-2.678294000	-1.840709000	1.208771000
6	-2.879183000	-0.458390000	0.707359000
6	-1.800067000	0.106999000	0.033966000
5	-0.360765000	-0.657732000	-0.108453000
6	-2.980184000	-2.021379000	2.651091000
1	-2.443316000	-1.256489000	3.209590000
1	-4.053995000	-1.924656000	2.809808000

1	-2.642722000	-3.012267000	2.955616000
6	-3.360562000	-2.833296000	0.331938000
1	-3.118139000	-3.839682000	0.676326000
1	-4.435987000	-2.660036000	0.379276000
1	-2.996925000	-2.671765000	-0.683598000
6	0.545286000	-0.120174000	1.135324000
6	0.628312000	-0.821485000	2.329659000
6	1.162589000	1.126773000	1.150789000
6	1.309613000	-0.370367000	3.453307000
6	1.865112000	1.620690000	2.240685000
6	1.941686000	0.862263000	3.402645000
6	0.241644000	-0.498613000	-1.607399000
6	1.553181000	-0.194019000	-1.955767000
6	-0.595916000	-0.775187000	-2.686178000
6	1.995177000	-0.115714000	-3.273092000
6	-0.200841000	-0.712437000	-4.014165000
6	1.111824000	-0.371905000	-4.309980000
9	1.347270000	-1.098532000	4.571419000
9	-0.014554000	-2.012077000	2.468562000
9	2.600815000	1.323526000	4.463322000
9	2.449487000	2.816973000	2.196134000
9	1.082678000	1.920927000	0.073188000
9	2.483749000	0.019082000	-1.015567000
9	3.263978000	0.189825000	-3.546203000
9	1.520136000	-0.306496000	-5.575937000
9	-1.057478000	-0.986455000	-5.000224000
9	-1.871171000	-1.154600000	-2.460746000
1	-1.657728000	-1.991761000	1.066908000
1	-0.498340000	-1.869722000	0.033358000
6	-2.021877000	1.404889000	-0.453327000
1	-1.211515000	1.902780000	-0.978202000
6	-3.235874000	2.059229000	-0.282012000
1	-3.368567000	3.062205000	-0.675002000
6	-4.114727000	0.154101000	0.891133000
1	-4.926964000	-0.347695000	1.410291000
6	-4.289427000	1.436631000	0.388988000
1	-5.238443000	1.944804000	0.519435000

4. FLP-H^+/H^- + CO2 (TS)

H

E(RM062X) = -581.329561120

6	-1.271530000	1.645108000	0.674664000
6	0.079992000	1.830781000	0.981503000
5	1.233439000	0.729497000	0.754548000
8	1.693080000	-2.112693000	2.052522000
6	0.735876000	-1.538438000	1.657755000
8	-0.416712000	-1.675712000	1.264488000
6	-1.581091000	0.283872000	-1.343294000
1	-0.580047000	0.599768000	-1.631781000
1	-1.765902000	-0.737680000	-1.679487000
1	-2.329899000	0.965190000	-1.750964000
6	-2.969862000	-0.190804000	0.630626000
1	-3.027709000	-1.249081000	0.374801000
1	-3.001415000	-0.072242000	1.712693000
1	-3.789368000	0.353419000	0.161341000
7	-1.663478000	0.319513000	0.141495000
1	-0.977630000	-0.401033000	0.527932000
1	1.006112000	-0.165806000	1.710907000
1	1.159402000	0.119493000	-0.286272000
1	2.336242000	1.102519000	1.041746000
6	0.405159000	3.104378000	1.473916000
1	1.440888000	3.297530000	1.736055000
6	-0.541886000	4.112223000	1.627885000
1	-0.243708000	5.082581000	2.011983000
6	-2.244160000	2.630128000	0.803389000
1	-3.279960000	2.440021000	0.540077000
6	-1.871626000	3.879278000	1.288561000
1	-2.617252000	4.658773000	1.401811000

Mes'

E(RM062X) = -1279.23019274

7	-1.181653000	1.513919000	1.071874000
6	-0.942199000	2.167130000	-0.239640000
6	0.327033000	2.121658000	-0.838490000
5	1.719979000	1.680233000	-0.113665000
6	2.954906000	1.360775000	-1.068594000
6	2.686027000	0.532844000	-2.174451000
6	4.295614000	1.758912000	-0.876196000
6	3.648820000	0.113285000	-3.085285000
6	5.259941000	1.353245000	-1.804289000
6	4.970268000	0.546500000	-2.900776000
6	1.871998000	2.365604000	1.330142000
6	1.952078000	1.625148000	2.517335000
6	1.874971000	3.772867000	1.444795000
6	2.013154000	2.210276000	3.784154000
6	1.948474000	4.358922000	2.709786000
6	2.006540000	3.608666000	3.884469000
6	4.764867000	2.593174000	0.294326000
1	4.519876000	2.122246000	1.249479000
1	5.848507000	2.726408000	0.247904000
1	4.308741000	3.587072000	0.307905000
6	6.054762000	0.131252000	-3.859143000
1	6.158501000	-0.958810000	-3.892737000
1	5.832698000	0.460060000	-4.880410000
1	7.019169000	0.553974000	-3.569761000
6	1.796912000	4.671928000	0.231660000
1	0.761837000	4.803503000	-0.105891000
1	2.203794000	5.661093000	0.457719000
1	2.355691000	4.258210000	-0.613915000
6	2.079058000	4.285341000	5.228252000
1	1.240938000	3.993755000	5.870811000
1	2.995807000	4.012010000	5.761805000
1	2.061922000	5.372138000	5.122933000
6	-2.360652000	0.597917000	1.050383000
1	-2.338709000	0.013250000	1.969585000
1	-3.283043000	1.173648000	0.985304000
1	-2.257001000	-0.070830000	0.198194000
6	-1.288605000	2.483730000	2.197798000
1	-2.212431000	3.053554000	2.079424000
1	-1.307955000	1.919342000	3.131540000
1	-0.425096000	3.146658000	2.183721000
6	0.400809000	2.728359000	-2.105780000
1	1.358879000	2.718383000	-2.615861000
6	-0.678959000	3.360107000	-2.711662000
1	-0.558846000	3.818847000	-3.687760000
6	-2.035749000	2.809116000	-0.816145000
1	-2.993240000	2.838868000	-0.305366000
6	-1.905183000	3.416021000	-2.058390000
1	-2.755362000	3.916812000	-2.508744000
1	6.289619000	1.673822000	-1.656539000
1	1.962557000	5.445420000	2.783779000
1	1.949829000	0.539718000	2.464678000
6	2.091105000	1.352226000	5.020280000
1	1.261710000	1.558056000	5.706421000
1	2.061762000	0.291922000	4.762113000
1	3.015404000	1.539422000	5.577812000
1	1.666758000	0.176435000	-2.316555000
6	3.286619000	-0.792539000	-4.232627000
1	2.221542000	-1.032052000	-4.217729000
1	3.520120000	-0.332673000	-5.199599000
1	3.841864000	-1.735583000	-4.184976000
8	0.112629000	-0.696418000	1.346082000

6	0.979479000	-0.812241000	0.458820000
8	1.444842000	-1.667473000	-0.239814000
1	1.503057000	0.296525000	0.254044000
1	-0.400503000	0.804160000	1.271849000

Mes

E(RM062X) = -1279.22009947

7	-1.231755000	1.288828000	1.114435000
6	-1.057631000	2.001292000	-0.174528000
6	0.200154000	2.078389000	-0.784650000
5	1.637376000	1.703986000	-0.120954000
6	2.829636000	1.396387000	-1.146807000
6	2.655526000	0.433738000	-2.173588000
6	4.099921000	2.028384000	-1.060621000
6	3.713540000	0.102796000	-3.025064000
6	5.122165000	1.682012000	-1.942739000
6	4.958026000	0.707876000	-2.924715000
6	1.869653000	2.399278000	1.320720000
6	2.533205000	1.732638000	2.378506000
6	1.425868000	3.723702000	1.578764000
6	2.589236000	2.301185000	3.654078000
6	1.527068000	4.271756000	2.859849000
6	2.069209000	3.560581000	3.927450000
6	4.429109000	3.110214000	-0.053524000
1	4.534494000	2.710051000	0.958911000
1	5.373036000	3.589968000	-0.323437000
1	3.660265000	3.884283000	-0.006182000
6	6.097585000	0.319031000	-3.829850000
1	5.733861000	-0.157655000	-4.743210000
1	6.695096000	1.190430000	-4.110999000
1	6.766509000	-0.389297000	-3.329865000
6	0.898857000	4.650268000	0.498955000
1	-0.163541000	4.496488000	0.277342000
1	1.022529000	5.688524000	0.816964000
1	1.439459000	4.523773000	-0.442358000
6	2.167979000	4.162741000	5.305369000
1	1.907154000	3.431637000	6.075395000
1	3.188088000	4.502732000	5.511387000
1	1.503594000	5.023666000	5.411041000
6	-2.247604000	0.199134000	1.016146000
1	-2.174307000	-0.405269000	1.919380000
1	-3.244032000	0.628210000	0.914102000
1	-2.004985000	-0.415230000	0.150264000
6	-1.529089000	2.190709000	2.260584000
1	-2.497219000	2.668077000	2.099900000
1	-1.552440000	1.583799000	3.167087000
1	-0.737565000	2.934958000	2.335616000
6	0.211305000	2.707971000	-2.043056000
1	1.163338000	2.774733000	-2.563234000
6	-0.920807000	3.266993000	-2.620996000
1	-0.852015000	3.753586000	-3.588560000
6	-2.208605000	2.562444000	-0.726067000
1	-3.160343000	2.496847000	-0.206818000
6	-2.140354000	3.210779000	-1.951794000
1	-3.032853000	3.652276000	-2.381752000
1	6.081397000	2.189401000	-1.859461000
1	1.185232000	5.292486000	3.023514000
8	0.364606000	-0.656212000	1.690404000
6	1.172554000	-0.790161000	0.751600000
8	1.788898000	-1.664982000	0.210701000
1	1.395551000	0.325356000	0.250279000
1	-0.356634000	0.722071000	1.373072000
6	1.348825000	-0.270614000	-2.480408000
1	0.871081000	0.191299000	-3.352747000
1	1.541271000	-1.319832000	-2.715724000
1	0.626306000	-0.246946000	-1.669289000
6	3.293292000	0.437272000	2.195192000
1	4.257511000	0.516324000	2.706268000
1	2.759631000	-0.408765000	2.639080000
1	3.493188000	0.206306000	1.147618000
1	3.550093000	-0.651511000	-3.792829000
1	3.087005000	1.747862000	4.449211000

FMes

E(RM062X) = -3065.65162653

7	-1.200210000	1.226169000	1.017854000
6	-0.999282000	2.030433000	-0.199188000
6	0.276565000	2.240863000	-0.750076000
5	1.716085000	1.907686000	-0.124484000
6	2.856712000	1.483857000	-1.199513000
6	2.616957000	0.458339000	-2.149619000
6	4.166688000	2.029398000	-1.221835000
6	3.620687000	0.005234000	-3.011969000
6	5.157520000	1.579034000	-2.084410000
6	4.885700000	0.553466000	-2.974485000
6	1.990500000	2.536868000	1.363354000
6	2.639919000	1.842271000	2.410143000
6	1.458483000	3.799648000	1.747873000
6	2.590243000	2.257543000	3.740922000
6	1.439169000	4.231733000	3.072667000
6	1.953919000	3.434336000	4.080744000
6	4.610302000	3.149276000	-0.301780000
6	5.949851000	0.100307000	-3.934857000
6	0.854939000	4.833871000	0.805752000
6	1.820427000	3.856034000	5.516943000
6	-2.215766000	0.158414000	0.808286000
1	-2.169996000	-0.520372000	1.661198000
1	-3.221302000	0.574644000	0.723897000
1	-1.958961000	-0.388292000	-0.099218000
6	-1.555793000	2.044549000	2.198967000
1	-2.531012000	2.519406000	2.054353000
1	-1.589927000	1.390082000	3.072934000
1	-0.800735000	2.813385000	2.346079000
6	0.307076000	2.916266000	-1.982807000
1	1.269356000	3.079671000	-2.458662000
6	-0.829767000	3.422356000	-2.598500000
1	-0.745110000	3.948673000	-3.543036000
6	-2.145957000	2.542958000	-0.801177000
1	-3.116658000	2.386881000	-0.341825000
6	-2.067349000	3.250170000	-1.993791000
1	-2.968945000	3.645148000	-2.449466000
1	6.144379000	2.024325000	-2.059898000
1	1.025923000	5.202933000	3.317937000
8	0.383505000	-0.548247000	1.621780000
6	1.300708000	-0.660751000	0.749913000
8	1.928795000	-1.565420000	0.291922000
1	1.562894000	0.423661000	0.321319000
1	-0.259084000	0.454286000	1.349446000
6	1.285830000	-0.207639000	-2.507495000
6	3.537289000	0.621431000	2.266427000
1	3.407457000	-0.790744000	-3.714682000
1	3.082602000	1.666520000	4.505606000
9	5.734316000	3.731165000	-0.745242000
9	3.693990000	4.119428000	-0.208547000
9	4.874565000	2.724061000	0.943332000
9	7.156488000	0.092805000	-3.354237000
9	6.027858000	0.920629000	-4.992856000
9	5.705722000	-1.129859000	-4.399957000
9	1.482246000	-1.481513000	-2.869247000
9	0.759940000	0.421389000	-3.574039000
9	0.323649000	-0.239043000	-1.575839000
9	0.636565000	3.475505000	6.021008000
9	2.772749000	3.313204000	6.282732000
9	1.892547000	5.186832000	5.644875000

9	3.848622000	0.295484000	1.013173000
9	4.694448000	0.849427000	2.907544000
9	2.985358000	-0.453727000	2.847048000
9	1.359156000	4.821592000	-0.426483000
9	-0.480564000	4.698420000	0.705700000
9	1.064796000	6.072521000	1.282933000

CF_3

E(RM062X) = -1255.43875211

6	-1.241041000	1.634325000	0.458262000
6	0.090618000	1.854878000	0.842903000
5	1.266881000	0.808495000	0.756721000
8	1.308295000	-2.298653000	1.975227000
6	0.616108000	-1.580797000	1.336794000
8	-0.322451000	-1.770477000	0.486574000
6	-2.300847000	0.165287000	-1.190549000
1	-1.609547000	0.592252000	-1.914026000
1	-2.441627000	-0.896310000	-1.411280000
1	-3.269519000	0.672720000	-1.255835000
6	-2.684413000	-0.166298000	1.185441000
1	-2.934021000	-1.212577000	0.994114000
1	-2.222596000	-0.083467000	2.171295000
1	-3.598624000	0.435886000	1.166301000
7	-1.716380000	0.283983000	0.161048000
1	-0.815939000	-0.813674000	0.255844000
1	0.765554000	-0.392331000	1.515365000
6	0.442945000	3.165569000	1.212054000
1	1.461106000	3.371027000	1.523832000
6	-0.469309000	4.213006000	1.163520000
1	-0.158886000	5.213383000	1.445211000
6	-2.161360000	2.679725000	0.415543000
1	-3.188418000	2.485791000	0.120424000
6	-1.776551000	3.971053000	0.757211000
1	-2.499951000	4.778569000	0.716837000
6	2.550966000	1.004142000	1.713513000
9	2.207654000	1.299652000	2.983682000
9	3.334287000	-0.083260000	1.760135000
9	3.322022000	2.027416000	1.274653000
6	1.656692000	0.238575000	-0.702002000
9	2.450334000	1.145973000	-1.303530000
9	2.324983000	-0.926204000	-0.683689000
9	0.594794000	0.055281000	-1.524436000

PFtB

E(RM062X) = -2682.18017191

7	-0.928010000	0.375372000	-0.414159000
6	-0.963165000	1.829335000	-0.498009000
6	0.092690000	2.649419000	-0.056441000
5	1.554724000	2.343531000	0.569005000
6	2.797360000	2.372040000	-0.621123000
6	2.166291000	1.990450000	-1.989303000
6	3.993164000	1.379994000	-0.453635000
6	1.647434000	2.726789000	2.246652000
6	2.936463000	2.287265000	2.998402000
6	0.456063000	2.076251000	3.004259000
6	3.439377000	3.774716000	-0.814087000
9	4.293073000	4.023773000	0.177191000
9	4.104096000	3.863603000	-1.968572000
9	2.532676000	4.753908000	-0.849683000
6	1.528130000	4.261866000	2.501476000
9	1.965921000	4.622854000	3.704934000
9	2.251327000	4.947347000	1.609179000
9	0.261263000	4.677279000	2.419686000
9	4.433821000	1.320481000	0.790998000
9	5.034410000	1.714879000	-1.217755000
9	3.622009000	0.148251000	-0.828746000
9	3.089539000	1.689686000	-2.902926000
9	1.424870000	2.978165000	-2.489651000
9	1.383627000	0.904990000	-1.863885000
9	3.964452000	3.026958000	2.574180000
9	3.192765000	1.002768000	2.808070000
9	2.852581000	2.446763000	4.322851000
9	-0.727406000	2.318764000	2.434741000
9	0.366814000	2.523054000	4.256951000
9	0.600518000	0.743341000	3.052135000
1	0.265468000	-0.352104000	-0.159919000
1	1.746034000	0.607575000	0.887234000
6	-2.137814000	2.377007000	-1.018611000
1	-2.936103000	1.709898000	-1.327164000
6	-2.309887000	3.745104000	-1.149996000
1	-3.229285000	4.145566000	-1.563090000
6	-0.124288000	4.035476000	-0.203058000
1	0.639645000	4.734501000	0.096340000
6	-1.282488000	4.580207000	-0.739570000
1	-1.370970000	5.657477000	-0.828009000
6	1.866891000	-0.587993000	0.878647000
8	2.731104000	-1.089127000	1.518687000
8	0.978683000	-1.112383000	0.112309000
6	-1.776390000	-0.133549000	0.684421000
1	-2.831465000	0.108321000	0.512489000
1	-1.655587000	-1.218273000	0.737591000
1	-1.454537000	0.307949000	1.625608000
6	-1.295773000	-0.291803000	-1.682294000
1	-0.776748000	0.193726000	-2.507119000
1	-0.974903000	-1.335520000	-1.619918000
1	-2.375693000	-0.270731000	-1.861060000

C_6F_5

E(RM062X) = -2035.73872997

7	-1.313361000	1.339904000	0.964398000
6	-1.082708000	2.082993000	-0.288233000
6	0.206464000	2.218350000	-0.820322000
5	1.577545000	1.809793000	-0.112270000
6	2.785125000	1.377602000	-1.050594000
6	2.592418000	0.381183000	-2.008613000
6	4.075245000	1.896006000	-0.967140000
6	3.603272000	-0.080965000	-2.837660000
6	5.112164000	1.465299000	-1.783768000
6	4.872090000	0.471848000	-2.723298000
6	1.900595000	2.450287000	1.311381000
6	2.851893000	1.878234000	2.159345000
6	1.299019000	3.608183000	1.797215000
6	3.164960000	2.382120000	3.410885000
6	1.580778000	4.146246000	3.047736000
6	2.520943000	3.530135000	3.858051000
6	-2.216088000	0.176717000	0.746825000
1	-2.242081000	-0.408792000	1.666816000
1	-3.220874000	0.510744000	0.482201000
1	-1.804087000	-0.433090000	-0.057893000
6	-1.825794000	2.201293000	2.059765000
1	-2.869912000	2.467872000	1.876326000
1	-1.748221000	1.642812000	2.995240000
1	-1.226085000	3.107896000	2.109321000
6	0.303560000	2.893129000	-2.046930000
1	1.284797000	3.005930000	-2.498587000
6	-0.802621000	3.435409000	-2.691464000
1	-0.679254000	3.956517000	-3.634884000
6	-2.200638000	2.620810000	-0.919430000
1	-3.186492000	2.507178000	-0.478200000
6	-2.063135000	3.305899000	-2.121177000
1	-2.937454000	3.724501000	-2.607653000
8	0.365731000	-0.193949000	1.939849000
6	1.184081000	-0.524186000	1.030864000
8	1.878661000	-1.467624000	0.797743000

1	1.240694000	0.351656000	0.208755000
1	-0.375347000	0.746851000	1.427423000
9	4.071056000	1.789860000	4.181182000
9	3.493115000	0.775484000	1.769996000
9	2.803455000	4.030439000	5.053647000
9	0.952297000	5.243943000	3.465667000
9	0.385771000	4.273697000	1.071926000
9	4.364557000	2.858190000	-0.084814000
9	6.327004000	1.998313000	-1.679520000
9	5.853566000	0.052630000	-3.512079000
9	3.372096000	-1.034499000	-3.735576000
9	1.386317000	-0.181096000	-2.137915000

5. FLP-H^+/H^- + HCOOH (TS)

H

E(RM062X) = -582.505333205

7	-1.635997000	1.808916000	0.948735000
6	-1.109879000	2.241146000	-0.361723000
6	0.277651000	2.171351000	-0.556900000
5	1.351764000	1.685712000	0.538189000
6	-2.989328000	1.213230000	0.909070000
1	-3.165739000	0.728734000	1.870647000
1	-3.752260000	1.975242000	0.738634000
1	-3.013331000	0.463672000	0.118958000
6	-1.565436000	2.898276000	1.949580000
1	-2.259546000	3.693132000	1.663388000
1	-1.837470000	2.496820000	2.927959000
1	-0.546872000	3.279575000	1.976003000
6	0.725174000	2.601126000	-1.816272000
1	1.792427000	2.561014000	-2.013338000
6	-0.134732000	3.074849000	-2.802237000
1	0.260207000	3.395184000	-3.761315000
6	-1.993701000	2.725184000	-1.321590000
1	-3.060092000	2.775561000	-1.127949000
6	-1.501603000	3.142161000	-2.554273000
1	-2.185003000	3.514114000	-3.310380000
1	2.493193000	1.901378000	0.223956000
1	1.091955000	1.948375000	1.690081000
1	-1.007584000	0.885859000	1.243955000
1	1.310558000	0.372192000	0.518036000
6	0.660690000	-0.629506000	1.304233000
8	1.092189000	-1.748410000	0.670005000
8	-0.594873000	-0.399164000	1.293807000
1	0.396463000	-1.972937000	0.035318000
1	1.270125000	-0.447167000	2.195028000

Mes'

E(RM062X) = -1280.40568129

7	-1.585606000	1.264352000	0.066496000
6	-1.085120000	2.300401000	-0.863583000
6	0.286822000	2.582562000	-0.874667000
5	1.467018000	1.974432000	0.072653000
6	2.699493000	1.478508000	-0.844360000
6	2.432689000	0.412235000	-1.723035000
6	3.995749000	2.022665000	-0.880482000
6	3.379165000	-0.158005000	-2.569531000
6	4.949571000	1.457280000	-1.736602000
6	4.678819000	0.375498000	-2.567926000
6	1.799219000	2.662475000	1.499346000
6	2.573588000	1.864138000	2.362950000
6	1.393468000	3.918830000	1.993411000
6	2.957303000	2.245932000	3.645193000
6	1.776292000	4.304008000	3.284185000
6	2.545849000	3.501386000	4.120162000
6	4.404931000	3.220490000	-0.052417000
1	4.607690000	2.946587000	0.987635000
1	5.307480000	3.678205000	-0.466511000
1	3.618019000	3.979506000	-0.022939000
6	5.745210000	-0.196698000	-3.464854000
1	5.928608000	-1.254404000	-3.245091000
1	5.456203000	-0.137996000	-4.520211000
1	6.688699000	0.339867000	-3.343893000
6	0.586859000	4.905389000	1.178157000
1	-0.370307000	4.493152000	0.842335000
1	0.379213000	5.803945000	1.764815000
1	1.122061000	5.211268000	0.273932000
6	2.932554000	3.968002000	5.499007000
1	2.560435000	3.286621000	6.272274000
1	4.021083000	4.012877000	5.615017000
1	2.531005000	4.962732000	5.704519000
6	-2.884491000	0.651636000	-0.294322000
1	-2.995256000	-0.246904000	0.314482000
1	-3.709566000	1.338196000	-0.096430000
1	-2.864604000	0.375539000	-1.348121000
6	-1.615959000	1.750533000	1.471174000
1	-2.363500000	2.543087000	1.557729000
1	-1.879212000	0.911347000	2.119315000
1	-0.631420000	2.136870000	1.741039000
6	0.688409000	3.539487000	-1.823486000
1	1.752048000	3.750930000	-1.907886000
6	-0.203462000	4.216575000	-2.644804000
1	0.160717000	4.954655000	-3.352380000
6	-2.005907000	2.967216000	-1.672332000
1	-3.063943000	2.735333000	-1.627045000
6	-1.564181000	3.938865000	-2.561244000
1	-2.278132000	4.457331000	-3.192191000
1	5.949626000	1.888234000	-1.757966000
1	1.462648000	5.280634000	3.650059000
1	2.913258000	0.894793000	1.994718000
6	3.797908000	1.336130000	4.503172000
1	3.292650000	1.089632000	5.443849000
1	4.016663000	0.401898000	3.981871000
1	4.751285000	1.805705000	4.770132000
1	1.413879000	0.015052000	-1.752809000
6	3.018858000	-1.304939000	-3.478772000
1	1.974274000	-1.596913000	-3.345553000
1	3.160825000	-1.040560000	-4.532632000
1	3.644148000	-2.184386000	-3.287725000
8	-0.234572000	-0.862385000	0.207709000
6	0.753909000	-0.533011000	0.937221000
8	1.940297000	-1.146436000	0.806138000
1	1.018024000	0.827907000	0.523961000
1	-0.915981000	0.356629000	0.058383000
1	0.629209000	-0.220005000	1.986657000
1	2.064857000	-1.364152000	-0.132306000

Mes

E(RM062X) = -1280.39393719

7	-1.659059000	1.618362000	0.301176000
6	-1.076217000	2.525071000	-0.710213000
6	0.315521000	2.575133000	-0.888482000
5	1.523011000	1.851102000	-0.045789000
6	2.739156000	1.434388000	-1.033328000
6	2.526060000	0.457335000	-2.034023000
6	4.033768000	2.002487000	-0.957013000
6	3.582997000	-0.007020000	-2.819770000
6	5.065414000	1.526566000	-1.769498000
6	4.871727000	0.497758000	-2.686684000
6	1.883856000	2.427319000	1.436836000
6	2.641942000	1.615682000	2.319622000
6	1.473664000	3.691407000	1.944361000
6	2.852529000	1.995111000	3.649846000
6	1.713980000	4.040911000	3.274733000

6	2.376221000	3.194474000	4.160361000
6	4.364952000	3.174578000	-0.055763000
1	4.531583000	2.874981000	0.983262000
1	5.272401000	3.669692000	-0.411657000
1	3.560098000	3.914213000	-0.041019000
6	6.013944000	-0.040865000	-3.508802000
1	6.746369000	0.740207000	-3.729170000
1	6.538450000	-0.840603000	-2.974892000
1	5.660240000	-0.455341000	-4.456389000
6	0.825900000	4.764513000	1.090951000
1	-0.196369000	4.523337000	0.783439000
1	0.790852000	5.704997000	1.646139000
1	1.389035000	4.940872000	0.171064000
6	2.575841000	3.574728000	5.604371000
1	3.438278000	3.058983000	6.033674000
1	2.732330000	4.651334000	5.712327000
1	1.699836000	3.309433000	6.206163000
6	-3.010801000	1.102517000	-0.021611000
1	-3.183544000	0.235861000	0.618498000
1	-3.776431000	1.857391000	0.165809000
1	-3.030376000	0.793376000	-1.066210000
6	-1.636928000	2.188109000	1.671613000
1	-2.261282000	3.085000000	1.702291000
1	-2.025113000	1.433390000	2.358949000
1	-0.609310000	2.435096000	1.939867000
6	0.741650000	3.435197000	-1.919061000
1	1.806937000	3.478041000	-2.130443000
6	-0.120831000	4.232526000	-2.661194000
1	0.273291000	4.883716000	-3.434983000
6	-1.963022000	3.324059000	-1.432677000
1	-3.030470000	3.273471000	-1.248127000
6	-1.486753000	4.190945000	-2.407462000
1	-2.179622000	4.808777000	-2.968604000
1	6.051116000	1.981830000	-1.687545000
1	1.385145000	5.016984000	3.627412000
8	-0.669208000	-0.646333000	0.528730000
6	0.561843000	-0.591603000	0.864545000
8	1.393956000	-1.529620000	0.367297000
1	1.046466000	0.637502000	0.300900000
1	-1.091643000	0.635369000	0.369319000
1	0.873340000	-0.295486000	1.876437000
1	0.964672000	-1.880380000	-0.427716000
1	3.388255000	-0.772767000	-3.569475000
6	1.147838000	-0.061092000	-2.393664000
1	0.710569000	0.570486000	-3.176309000
1	1.210441000	-1.076016000	-2.801157000
1	0.433439000	-0.056987000	-1.570235000
6	3.381075000	0.365126000	1.883021000
1	4.442724000	0.607598000	1.750117000
1	3.323789000	-0.410965000	2.653279000
1	3.044938000	-0.056234000	0.940632000
1	3.429422000	1.334279000	4.295430000

FMes

E(RM062X) = -3066.82658646

7	-1.709081000	1.904376000	0.412759000
6	-1.100135000	2.761641000	-0.613709000
6	0.283494000	2.756388000	-0.855251000
5	1.487573000	1.973998000	-0.085489000
6	2.597944000	1.440081000	-1.167491000
6	2.250711000	0.412723000	-2.076229000
6	3.952094000	1.863409000	-1.247437000
6	3.199400000	-0.245872000	-2.862640000
6	4.895729000	1.211328000	-2.033176000
6	4.528369000	0.120835000	-2.805499000
6	1.916753000	2.468146000	1.433646000
6	2.608403000	1.619426000	2.341694000
6	1.483301000	3.687727000	2.022111000
6	2.658889000	1.858642000	3.715509000
6	1.524935000	3.924974000	3.395181000
6	2.057656000	2.980428000	4.254174000
6	4.441495000	3.164071000	-0.637322000
6	5.569387000	-0.632134000	-3.583139000
6	1.083964000	4.913439000	1.215525000
6	2.014293000	3.192760000	5.739880000
6	-2.933903000	1.211447000	-0.052680000
1	-3.154262000	0.411330000	0.656871000
1	-3.788688000	1.889744000	-0.106587000
1	-2.735214000	0.779842000	-1.033477000
6	-1.964156000	2.615623000	1.683284000
1	-1.025146000	3.005702000	2.071898000
1	-2.660045000	3.444998000	1.521897000
1	-2.387636000	1.904761000	2.396218000
6	0.702843000	3.569821000	-1.923975000
1	1.758040000	3.593116000	-2.172950000
6	-0.156536000	4.381205000	-2.654604000
1	0.234783000	4.993797000	-3.459900000
6	-1.973676000	3.581773000	-1.324935000
1	-3.032860000	3.579870000	-1.089662000
6	-1.508502000	4.401208000	-2.344514000
1	-2.199514000	5.032194000	-2.893161000
1	5.918711000	1.564276000	-2.059362000
1	1.173073000	4.869905000	3.791242000
8	-0.681929000	-0.358816000	1.028826000
6	0.606227000	-0.428645000	0.919991000
8	1.099908000	-1.404859000	0.134097000
1	0.993508000	0.737174000	0.341990000
1	-1.032379000	0.810740000	0.742870000
1	1.221406000	-0.304245000	1.818072000
1	0.373413000	-1.684876000	-0.444111000
1	2.892289000	-1.042861000	-3.529391000
6	0.843351000	-0.002304000	-2.475584000
6	3.545395000	0.484860000	1.951295000
1	3.185416000	1.167724000	4.363543000
9	5.032812000	-1.287665000	-4.621239000
9	6.192497000	-1.539531000	-2.819018000
9	6.512422000	0.191691000	-4.061457000
9	0.492913000	0.629871000	-3.602736000
9	-0.150363000	0.210200000	-1.597180000
9	0.789595000	-1.326478000	-2.741180000
9	4.257773000	3.283582000	0.680906000
9	3.814057000	4.201017000	-1.219505000
9	5.753700000	3.347967000	-0.847098000
9	1.807242000	5.023444000	0.101818000
9	1.309745000	6.033478000	1.925678000
9	-0.216686000	4.959105000	0.881027000
9	3.296445000	-0.112066000	0.785163000
9	3.522545000	-0.491260000	2.880305000
9	4.805361000	0.938696000	1.897020000
9	2.082495000	4.493434000	6.052550000
9	0.872896000	2.721837000	6.265478000
9	3.022513000	2.566024000	6.358529000

CF_3

E(RM062X) = -1256.63240007

7	-1.719780000	1.695177000	0.879406000
6	-1.133706000	2.286663000	-0.329221000
6	0.258422000	2.277091000	-0.523186000
5	1.356307000	1.685453000	0.480309000
6	-2.942790000	0.909179000	0.611518000
1	-3.190600000	0.350263000	1.517143000
1	-3.793918000	1.543894000	0.348655000
1	-2.744115000	0.204676000	-0.196586000
6	-2.012696000	2.745173000	1.879857000

1	-2.856881000	3.358226000	1.542341000
1	-2.261392000	2.269483000	2.831486000
1	-1.137463000	3.376897000	2.012259000
6	0.728235000	2.904228000	-1.690781000
1	1.794786000	2.924354000	-1.883197000
6	-0.120629000	3.510119000	-2.609887000
1	0.290737000	3.981441000	-3.496329000
6	-1.992498000	2.898426000	-1.242288000
1	-3.062675000	2.906401000	-1.063334000
6	-1.491447000	3.506620000	-2.386722000
1	-2.170298000	3.974017000	-3.092390000
1	-0.991773000	0.608016000	1.390282000
1	1.069456000	0.437470000	0.752629000
6	0.647518000	-0.561872000	1.591642000
8	1.140713000	-1.676182000	1.045546000
8	-0.648094000	-0.434192000	1.581426000
1	0.480157000	-2.009725000	0.419859000
1	1.236476000	-0.253110000	2.457654000
6	1.446662000	2.392391000	1.939026000
9	1.229526000	3.724226000	1.881914000
9	0.508326000	1.910828000	2.816251000
9	2.624763000	2.220813000	2.564685000
6	2.825983000	1.415060000	-0.131829000
9	3.543439000	2.552393000	-0.295507000
9	3.562215000	0.605695000	0.660111000
9	2.792162000	0.813237000	-1.343886000

PFtB

E(RM062X) = -2683.37056049

7	-1.070135000	0.340939000	0.001446000
6	-1.064502000	1.752179000	-0.330857000
6	0.059892000	2.590839000	-0.159978000
5	1.518734000	2.384065000	0.493758000
6	2.832068000	2.492079000	-0.595800000
6	2.329828000	2.412374000	-2.068317000
6	3.925969000	1.380638000	-0.510457000
6	1.588267000	2.757353000	2.171788000
6	2.721638000	2.093614000	2.999379000
6	0.239064000	2.293859000	2.800229000
6	3.592305000	3.837853000	-0.460158000
9	4.487495000	3.782894000	0.521613000
9	4.234437000	4.170037000	-1.579923000
9	2.750816000	4.847437000	-0.187835000
6	1.677505000	4.286561000	2.484026000
9	1.288167000	4.532208000	3.738634000
9	2.921776000	4.744414000	2.364456000
9	0.892689000	5.014687000	1.691233000
9	4.204700000	1.030355000	0.733836000
9	5.068144000	1.783797000	-1.074493000
9	3.529991000	0.287455000	-1.172181000
9	3.328154000	2.162271000	-2.919047000
9	1.770552000	3.557883000	-2.462059000
9	1.435662000	1.428790000	-2.222910000
9	3.929576000	2.462158000	2.598074000
9	2.624342000	0.755961000	2.910005000
9	2.656839000	2.405547000	4.295616000
9	-0.764834000	3.088224000	2.421432000
9	0.234137000	2.273398000	4.131361000
9	-0.041112000	1.047106000	2.409018000
1	-0.034292000	-0.585600000	1.043222000
1	1.748259000	0.466735000	0.648271000
6	-2.246628000	2.253547000	-0.885585000
1	-3.082583000	1.575581000	-1.023436000
6	-2.382540000	3.577152000	-1.269693000
1	-3.316933000	3.934595000	-1.689359000
6	-0.109449000	3.923728000	-0.593597000
1	0.712986000	4.617267000	-0.523900000
6	-1.293112000	4.420542000	-1.120048000
1	-1.346554000	5.461724000	-1.419009000
6	1.750352000	-0.712194000	0.573028000
8	2.930060000	-1.239863000	1.007719000
8	0.702370000	-1.185745000	1.310643000
6	-2.231991000	-0.051007000	0.815406000
1	-3.166073000	-0.089349000	0.239505000
1	-2.052479000	-1.052177000	1.222223000
1	-2.347664000	0.650157000	1.642027000
6	-0.998672000	-0.495788000	-1.204353000
1	-0.163657000	-0.171800000	-1.825454000
1	-0.837955000	-1.535269000	-0.900766000
1	-1.921257000	-0.436923000	-1.800244000
1	2.906187000	-1.223014000	1.973952000
1	1.669252000	-0.899857000	-0.504211000

C_6F_5

E(RM062X) = -2036.92541028

7	-1.631907000	1.273020000	0.272701000
6	-1.141607000	2.260105000	-0.697630000
6	0.233924000	2.514764000	-0.785883000
5	1.443002000	1.861816000	0.063687000
6	2.650800000	1.390430000	-0.893288000
6	2.413158000	0.400036000	-1.840874000
6	3.944278000	1.900665000	-0.888106000
6	3.371180000	-0.077553000	-2.720421000
6	4.937771000	1.459499000	-1.755802000
6	4.649451000	0.463471000	-2.676853000
6	1.870348000	2.587521000	1.438163000
6	2.829112000	1.988779000	2.255239000
6	1.352854000	3.788072000	1.917224000
6	3.271396000	2.531990000	3.450754000
6	1.768278000	4.370389000	3.111025000
6	2.735049000	3.740402000	3.879200000
6	-2.941192000	0.670840000	-0.047935000
1	-3.065788000	-0.204309000	0.593509000
1	-3.763834000	1.368183000	0.133496000
1	-2.943186000	0.354611000	-1.091127000
6	-1.650470000	1.826547000	1.645341000
1	-1.961555000	1.036126000	2.332700000
1	-0.648552000	2.163418000	1.909795000
1	-2.343229000	2.671431000	1.703521000
6	0.621265000	3.494457000	-1.712806000
1	1.681113000	3.713364000	-1.818138000
6	-0.287714000	4.192611000	-2.498502000
1	0.062613000	4.941973000	-3.200608000
6	-2.068949000	2.951020000	-1.477506000
1	-3.129064000	2.742254000	-1.391570000
6	-1.644032000	3.916899000	-2.382040000
1	-2.372338000	4.444679000	-2.988408000
8	-0.396961000	-0.826931000	0.597979000
6	0.817341000	-0.600590000	0.982622000
8	1.788855000	-1.360005000	0.466671000
1	1.051809000	0.682012000	0.525085000
1	-0.934003000	0.214171000	0.374894000
1	1.042910000	-0.349179000	2.027268000
1	1.460715000	-1.673702000	-0.391819000
9	3.081893000	-1.042313000	-3.593438000
9	5.588302000	0.029126000	-3.511506000
9	6.158758000	1.988703000	-1.714568000
9	4.288878000	2.876373000	-0.037969000
9	1.189533000	-0.167179000	-1.910443000
9	3.363576000	0.817011000	1.880577000
9	0.391670000	4.438853000	1.248043000
9	1.237708000	5.520105000	3.525120000
9	3.137069000	4.280593000	5.024639000
9	4.190523000	1.914699000	4.189674000

6. FLP-H^+/H^- + CH2(OH)2 (TS)

H

E(RM062X) = -583.629203977

6	-1.148309000	1.714891000	0.065057000
6	0.213378000	1.557897000	0.394779000
5	1.004274000	0.181607000	0.766789000
1	0.402805000	-2.710877000	0.569813000
1	-0.165316000	-2.938626000	-2.153956000
6	0.518971000	-2.529712000	-0.492272000
8	-0.448595000	-0.823710000	-1.610490000
8	-0.182428000	-3.288972000	-1.242727000
6	-3.217491000	0.639418000	-0.739614000
1	-2.972018000	0.999720000	-1.741085000
1	-3.668598000	-0.353982000	-0.822067000
1	-3.962790000	1.311098000	-0.289898000
6	-2.316363000	0.083189000	1.414793000
1	-2.778550000	-0.908949000	1.374072000
1	-1.401124000	0.028787000	2.001880000
1	-3.017226000	0.780450000	1.897094000
7	-1.996429000	0.528724000	0.053505000
1	-1.093721000	-0.440354000	-0.913638000
1	1.799061000	-0.079970000	-0.147180000
1	0.253859000	-0.154346000	-1.562405000
1	1.346591000	-1.923346000	-0.838884000
1	1.634259000	0.310523000	1.796335000
1	0.238652000	-0.778853000	0.908145000
6	0.977323000	2.736874000	0.378529000
1	2.032828000	2.653776000	0.627993000
6	0.455423000	3.984191000	0.055991000
1	1.095881000	4.861418000	0.053172000
6	-1.693831000	2.963576000	-0.251819000
1	-2.746824000	3.060092000	-0.494344000
6	-0.893587000	4.099853000	-0.262907000
1	-1.325246000	5.063511000	-0.514921000

Mes'

E(RM062X) = -1281.54491873

6	1.332228000	-0.616765000	-0.144615000
6	0.076514000	-1.200889000	-0.398367000
5	-1.333356000	-0.394418000	-0.560957000
1	-1.496204000	1.756317000	-2.475373000
1	-0.525363000	-0.113369000	-2.982560000
6	-0.421444000	1.732477000	-2.646980000
8	-0.104221000	3.045138000	-0.411765000
8	0.133431000	0.679348000	-3.030398000
6	1.576109000	1.110273000	1.502848000
1	0.746917000	0.636735000	2.033060000
1	1.524166000	2.194378000	1.653213000
1	2.524324000	0.736869000	1.920008000
6	2.552812000	1.439641000	-0.672253000
1	2.505058000	1.127429000	-1.718966000
1	3.548698000	1.184237000	-0.280263000
1	2.440641000	2.528132000	-0.615010000
7	1.456024000	0.818394000	0.069131000
1	0.254837000	2.144212000	-0.208060000
1	-0.967498000	3.055239000	0.017405000
1	0.190174000	2.626311000	-2.583788000
1	-1.070538000	0.803720000	-0.694682000
6	0.070839000	-2.608406000	-0.473838000
1	-0.879429000	-3.106371000	-0.650462000
6	1.211698000	-3.390900000	-0.345696000
1	1.142632000	-4.472498000	-0.415495000
6	2.489973000	-1.394913000	-0.014849000
1	3.441351000	-0.910915000	0.189565000
6	2.441285000	-2.777058000	-0.124154000
1	3.347428000	-3.366096000	-0.022554000
6	-2.118796000	-0.731431000	-1.967851000
6	-1.612237000	-1.601417000	-2.958749000
6	-3.286765000	-0.003591000	-2.332422000
6	-2.190021000	-1.781403000	-4.227278000
6	-3.858016000	-0.181131000	-3.591081000
6	-3.338217000	-1.055180000	-4.550722000
1	-4.751362000	0.388771000	-3.843217000
6	-2.214323000	-0.454467000	0.811998000
6	-3.104691000	-1.471892000	1.206101000
6	-2.055399000	0.608191000	1.717525000
6	-3.776620000	-1.371866000	2.430740000
6	-2.701108000	0.706257000	2.946833000
6	-3.594046000	-0.312027000	3.312894000
1	-4.472452000	-2.163109000	2.708638000
6	-4.001739000	-1.210225000	-5.893850000
1	-4.879258000	-0.565583000	-5.975414000
1	-3.318257000	-0.957486000	-6.711862000
1	-4.326043000	-2.243209000	-6.059454000
6	-3.933190000	0.964582000	-1.370589000
1	-3.197398000	1.645913000	-0.926329000
1	-4.708255000	1.553016000	-1.868211000
1	-4.381145000	0.434637000	-0.524926000
6	-3.364530000	-2.706017000	0.372068000
1	-2.683396000	-3.516439000	0.656184000
1	-4.383248000	-3.073429000	0.527583000
1	-3.229608000	-2.519363000	-0.695138000
6	-4.336080000	-0.255034000	4.622781000
1	-4.996796000	-1.117381000	4.736687000
1	-3.646509000	-0.245358000	5.474499000
1	-4.947733000	0.650963000	4.700620000
6	-1.586284000	-2.748132000	-5.211769000
1	-0.683997000	-3.209991000	-4.806004000
1	-2.291280000	-3.548384000	-5.462049000
1	-1.323005000	-2.253074000	-6.152985000
6	-2.457147000	1.881868000	3.857325000
1	-3.375376000	2.452680000	4.037570000
1	-2.087412000	1.561123000	4.837662000
1	-1.717020000	2.561694000	3.427153000
1	-1.378810000	1.417773000	1.440041000
1	-0.733814000	-2.201257000	-2.724598000

Mes

E(RM062X) = -1281.52334145

6	1.131382000	-1.518916000	0.019125000
6	-0.115415000	-1.702839000	-0.611651000
5	-1.258169000	-0.545222000	-0.789984000
1	-0.677866000	1.738090000	-2.398139000
1	1.230383000	0.702852000	-2.505677000
6	0.228588000	2.168402000	-1.977671000
8	0.370478000	2.244191000	0.433679000
8	1.357689000	1.613032000	-2.158172000
6	1.290975000	-0.227195000	2.061108000
1	0.251348000	-0.462488000	2.292633000
1	1.511863000	0.775944000	2.439951000
1	1.951372000	-0.951956000	2.561422000
6	2.848933000	0.204531000	0.295596000
1	2.931224000	1.272701000	0.522034000
1	3.056297000	0.051974000	-0.766141000
1	3.617125000	-0.327977000	0.875324000
7	1.485715000	-0.232800000	0.604938000
1	0.645075000	1.285308000	0.383369000
1	-0.465489000	2.195578000	0.920815000
1	0.264130000	3.167990000	-1.568367000
1	-0.609970000	0.485010000	-1.061802000
6	-0.340412000	-2.984142000	-1.150600000

1	-1.282241000	-3.158327000	-1.666997000
6	0.572537000	-4.026939000	-1.052183000
1	0.340702000	-4.997131000	-1.481684000
6	2.056774000	-2.564765000	0.129110000
1	3.001410000	-2.395308000	0.639191000
6	1.785323000	-3.819042000	-0.401061000
1	2.512773000	-4.619498000	-0.309310000
6	-2.179833000	-0.793075000	-2.136272000
6	-1.582265000	-0.739138000	-3.418799000
6	-3.584869000	-1.015477000	-2.127259000
6	-2.335673000	-0.809985000	-4.596417000
6	-4.311250000	-1.084582000	-3.316513000
6	-3.713501000	-0.960776000	-4.569564000
1	-5.385681000	-1.254203000	-3.263467000
6	-2.028897000	-0.087832000	0.586507000
6	-2.148508000	-0.886643000	1.752361000
6	-2.606514000	1.204748000	0.660921000
6	-2.696567000	-0.365638000	2.928421000
6	-3.149300000	1.699348000	1.851842000
6	-3.177129000	0.937752000	3.015037000
1	-2.766084000	-1.009771000	3.803787000
6	-4.533878000	-1.010663000	-5.832405000
1	-3.897673000	-1.115676000	-6.714640000
1	-5.233643000	-1.851170000	-5.816250000
1	-5.126355000	-0.097842000	-5.954505000
6	-4.373613000	-1.220417000	-0.851831000
1	-4.551545000	-0.282613000	-0.316922000
1	-5.344679000	-1.666069000	-1.083311000
1	-3.852661000	-1.881538000	-0.156738000
6	-1.757882000	-2.350284000	1.787533000
1	-2.197346000	-2.831554000	2.665229000
1	-2.108412000	-2.880380000	0.898548000
1	-0.674577000	-2.504209000	1.826323000
6	-3.722328000	1.489055000	4.306930000
1	-2.920030000	1.893548000	4.933583000
1	-4.435248000	2.296999000	4.123480000
1	-4.228517000	0.712350000	4.886259000
6	-0.079436000	-0.666776000	-3.637444000
1	0.474455000	-0.851370000	-2.711318000
1	0.240493000	-1.453029000	-4.327500000
1	0.216623000	0.278834000	-4.118349000
6	-2.723568000	2.108466000	-0.552067000
1	-2.819975000	1.534829000	-1.477086000
1	-3.606074000	2.747278000	-0.460368000
1	-1.859579000	2.777729000	-0.642685000
1	-1.823366000	-0.762640000	-5.557211000
1	-3.582443000	2.699018000	1.861110000

FMes

E(RM062X) = -3067.99065453

6	1.153954000	-1.866371000	-0.020870000
6	-0.169256000	-1.892434000	-0.508446000
5	-1.133339000	-0.585033000	-0.726033000
1	-0.661517000	2.195018000	-0.006888000
1	-0.451102000	2.768857000	-2.129725000
6	0.276429000	2.531429000	-0.442947000
8	0.514633000	1.371167000	1.837564000
8	0.375814000	2.944554000	-1.623137000
6	2.674925000	-0.810803000	1.594103000
1	2.234965000	-1.493779000	2.320660000
1	2.827034000	0.163414000	2.068845000
1	3.655886000	-1.199859000	1.287273000
6	2.447451000	0.090444000	-0.600809000
1	2.863055000	1.020247000	-0.191151000
1	1.764240000	0.318022000	-1.419056000
1	3.283569000	-0.498632000	-1.007618000
7	1.750830000	-0.630147000	0.467127000
1	0.771476000	0.540595000	1.349332000
1	0.109256000	1.057601000	2.651635000
1	1.164723000	2.589427000	0.179377000
1	-0.363515000	0.354612000	-0.987366000
6	-0.614660000	-3.143768000	-0.969316000
1	-1.624331000	-3.226143000	-1.356827000
6	0.156954000	-4.298472000	-0.938175000
1	-0.256064000	-5.236574000	-1.295695000
6	1.946876000	-3.018379000	-0.007171000
1	2.966871000	-2.964411000	0.359389000
6	1.456698000	-4.237745000	-0.454139000
1	2.086463000	-5.121362000	-0.428189000
6	-2.072978000	-0.858836000	-2.086034000
6	-1.561082000	-0.635451000	-3.393011000
6	-3.406240000	-1.333599000	-2.078981000
6	-2.319679000	-0.766807000	-4.550410000
6	-4.180952000	-1.464177000	-3.234786000
6	-3.647644000	-1.156815000	-4.469608000
1	-5.200638000	-1.822801000	-3.165663000
6	-2.057002000	0.080909000	0.499906000
6	-2.158529000	-0.381505000	1.843684000
6	-2.816270000	1.262402000	0.255396000
6	-2.932352000	0.252180000	2.812406000
6	-3.591583000	1.901048000	1.229882000
6	-3.651344000	1.396421000	2.509840000
1	-2.989319000	-0.153538000	3.814080000
6	-4.482552000	-1.223120000	-5.714218000
6	-4.146386000	-1.746556000	-0.822077000
6	-1.392260000	-1.579859000	2.387731000
6	-4.435017000	2.105005000	3.575502000
6	-0.125754000	-0.230179000	-3.635050000
6	-3.030482000	1.931086000	-1.092837000
1	-1.877029000	-0.577539000	-5.520598000
1	-4.167507000	2.784426000	0.981531000
9	-3.777007000	-1.690859000	-6.754553000
9	-5.552505000	-2.012461000	-5.556137000
9	-4.934073000	-0.009062000	-6.067506000
9	0.203813000	-0.289592000	-4.934204000
9	0.124261000	1.060656000	-3.272022000
9	0.757425000	-0.985125000	-2.984648000
9	-4.751808000	-0.713634000	-0.208628000
9	-3.355317000	-2.340419000	0.075320000
9	-5.122060000	-2.628198000	-1.104822000
9	-1.981397000	1.852600000	-1.967233000
9	-4.089300000	1.463652000	-1.744802000
9	-3.212672000	3.259676000	-0.947108000
9	-1.526412000	-2.703237000	1.700510000
9	-0.072507000	-1.296276000	2.469464000
9	-1.768197000	-1.869871000	3.648930000
9	-5.458625000	2.796887000	3.057417000
9	-4.929387000	1.247114000	4.476430000
9	-3.668809000	2.980495000	4.246502000

CF_3

E(RM062X) = -1257.79890042

6	2.727744000	-0.788217000	0.720170000
6	1.427126000	-1.148228000	0.330349000
5	0.329846000	-0.023855000	-0.005998000
1	-0.536398000	2.593245000	-0.464908000
1	-0.990401000	1.514847000	-2.266555000
6	-0.006957000	2.808647000	-1.390869000
8	1.630438000	2.971675000	0.643368000
8	-0.328375000	2.250687000	-2.467441000
6	3.774715000	1.019938000	1.979606000
1	3.174032000	0.692966000	2.830079000
1	3.841160000	2.112796000	1.993007000
1	4.791903000	0.613341000	2.080021000

6	3.896570000	0.969758000	-0.431922000
1	3.343357000	0.688053000	-1.331605000
1	4.873707000	0.462490000	-0.449034000
1	4.061135000	2.052626000	-0.438317000
7	3.104650000	0.614341000	0.745148000
1	1.999408000	2.051599000	0.666436000
1	1.142884000	3.019020000	1.474258000
1	0.778357000	3.557498000	-1.426116000
1	0.839787000	0.899602000	-0.621272000
6	1.127799000	-2.517444000	0.303644000
1	0.127823000	-2.834640000	0.022587000
6	2.066539000	-3.489204000	0.637561000
1	1.794615000	-4.539769000	0.608048000
6	3.677497000	-1.757169000	1.049109000
1	4.681246000	-1.454422000	1.334959000
6	3.349830000	-3.108099000	1.013558000
1	4.092881000	-3.854555000	1.276289000
6	-0.858476000	-0.556090000	-0.968000000
9	-1.730216000	0.525333000	-1.354467000
9	-0.434839000	-1.021422000	-2.155513000
9	-1.713510000	-1.456523000	-0.477500000
6	-0.325891000	0.556249000	1.359487000
9	-1.134222000	1.661866000	1.165412000
9	-1.107718000	-0.330033000	2.000617000
9	0.588128000	0.974820000	2.277377000

PFtB

E(RM062X) = -2684.53874871

6	2.583099000	-0.698408000	0.454583000
6	1.209896000	-1.009110000	0.568976000
5	-0.063496000	-0.059727000	0.140201000
1	-0.706058000	2.574260000	-1.258455000
1	1.042567000	2.338123000	-2.498332000
6	0.218216000	3.095529000	-1.025554000
8	1.908538000	3.068071000	0.953603000
8	1.210796000	3.001333000	-1.794431000
6	3.849200000	1.003114000	1.560813000
1	3.246083000	0.785763000	2.442857000
1	4.092799000	2.068364000	1.545364000
1	4.780750000	0.425276000	1.623357000
6	3.932183000	0.930212000	-0.816807000
1	3.461932000	0.572102000	-1.729299000
1	4.915727000	0.445500000	-0.726755000
1	4.096583000	2.010409000	-0.894472000
7	3.074284000	0.674347000	0.345869000
1	2.139631000	2.151426000	0.646438000
1	1.587716000	2.922303000	1.850881000
1	0.350527000	3.746419000	-0.168083000
1	0.319054000	1.059731000	-0.188041000
6	0.943819000	-2.317516000	1.019866000
1	-0.079491000	-2.591054000	1.231249000
6	1.913740000	-3.293943000	1.195793000
1	1.625923000	-4.284609000	1.532706000
6	3.562647000	-1.691241000	0.576952000
1	4.606002000	-1.422576000	0.435887000
6	3.241342000	-2.994887000	0.920071000
1	4.018384000	-3.747178000	1.010510000
6	-1.109164000	0.316809000	1.495783000
6	-0.699974000	-0.736647000	-1.417573000
6	-0.538174000	-2.266676000	-1.641089000
9	-1.147127000	-2.673052000	-2.769963000
9	0.754461000	-2.585734000	-1.774707000
9	-1.070476000	-3.001400000	-0.670452000
6	-2.156003000	-0.430009000	-1.819220000
9	-2.525173000	0.807062000	-1.467577000
9	-2.350764000	-0.494132000	-3.149741000
9	-2.998315000	-1.295433000	-1.259420000
6	0.162500000	-0.104822000	-2.523359000
9	1.432994000	0.108462000	-2.160555000
9	0.202903000	-0.764595000	-3.673462000
9	-0.310910000	1.151647000	-2.853470000
6	-2.368965000	-0.548146000	1.658662000
9	-3.371230000	-0.050216000	0.920925000
9	-2.163016000	-1.807648000	1.266464000
9	-2.809096000	-0.604144000	2.923104000
6	-0.288398000	0.185848000	2.802490000
9	-0.847461000	0.839446000	3.833071000
9	-0.159055000	-1.082891000	3.183385000
9	0.942623000	0.715616000	2.667663000
6	-1.596769000	1.784543000	1.521243000
9	-2.056300000	2.241807000	0.346576000
9	-2.578367000	1.992763000	2.401558000
9	-0.591310000	2.622392000	1.851641000

C_6F_5

E(RM062X) = -2038.07043438

6	1.026127000	-1.973995000	0.119495000
6	-0.131490000	-1.949912000	-0.677324000
5	-0.981181000	-0.595015000	-0.898752000
1	-0.635546000	2.228298000	-1.518330000
1	0.420125000	1.266423000	-3.216759000
6	0.442781000	2.288251000	-1.645831000
8	0.588274000	1.844169000	0.927167000
8	1.018769000	1.849680000	-2.678083000
6	1.831810000	-0.869615000	2.150175000
1	1.004795000	-1.356750000	2.668462000
1	1.974688000	0.134648000	2.562739000
1	2.753269000	-1.443824000	2.325160000
6	2.622468000	-0.190333000	-0.021876000
1	2.882131000	0.793435000	0.384085000
1	2.335165000	-0.084058000	-1.071928000
1	3.509256000	-0.840109000	0.028586000
7	1.492051000	-0.739176000	0.731113000
1	0.668776000	0.857758000	0.835240000
1	-0.170328000	1.975346000	1.507008000
1	1.063741000	2.814338000	-0.928737000
1	-0.174200000	0.302707000	-1.173573000
6	-0.509805000	-3.164630000	-1.262153000
1	-1.399704000	-3.193043000	-1.885936000
6	0.202683000	-4.345904000	-1.068206000
1	-0.134636000	-5.266812000	-1.533800000
6	1.754492000	-3.146422000	0.313234000
1	2.649940000	-3.132267000	0.928763000
6	1.342745000	-4.339011000	-0.274645000
1	1.911499000	-5.249436000	-0.114207000
6	-2.023815000	-0.715996000	-2.156019000
6	-1.690244000	-0.412588000	-3.464366000
6	-3.333293000	-1.171192000	-2.005499000
6	-2.542319000	-0.505398000	-4.555082000
6	-4.234995000	-1.288866000	-3.057168000
6	-3.838591000	-0.949709000	-4.344084000
6	-1.767660000	-0.022033000	0.418403000
6	-1.791305000	-0.597295000	1.685262000
6	-2.442244000	1.192201000	0.335332000
6	-2.394673000	0.002726000	2.789239000
6	-3.066151000	1.828984000	1.397053000
6	-3.038789000	1.222119000	2.647221000
9	-1.207309000	-1.777665000	1.925449000
9	-2.363315000	-0.590644000	3.981316000
9	-3.624154000	1.804591000	3.690234000
9	-3.682398000	3.000407000	1.234559000
9	-2.484817000	1.850431000	-0.852340000
9	-3.779754000	-1.539054000	-0.798898000
9	-0.415233000	0.007051000	-3.774478000

9	-2.131018000	-0.178063000	-5.779836000
9	-5.473482000	-1.726631000	-2.846099000
9	-4.687906000	-1.054135000	-5.361748000

7. FLP-H^+/H^- + CH2O (TS)

H

E(RM062X) = -507.257766658

7	-1.644322000	1.870811000	0.999740000
6	-1.106242000	2.239801000	-0.335684000
6	0.276715000	2.134588000	-0.517732000
5	1.333533000	1.640652000	0.600636000
6	-2.978981000	1.222182000	0.975201000
1	-3.158964000	0.800020000	1.964189000
1	-3.751741000	1.952385000	0.735654000
1	-2.947432000	0.420910000	0.239464000
6	-1.605034000	3.025971000	1.931671000
1	-2.273187000	3.800512000	1.550995000
1	-1.927572000	2.695567000	2.920584000
1	-0.580159000	3.390685000	1.970823000
6	0.727753000	2.523546000	-1.790885000
1	1.794309000	2.461344000	-1.986806000
6	-0.124803000	2.985558000	-2.786853000
1	0.274762000	3.272726000	-3.754624000
6	-1.989828000	2.718953000	-1.298494000
1	-3.054154000	2.797998000	-1.101717000
6	-1.491735000	3.090686000	-2.541413000
1	-2.167144000	3.456944000	-3.307151000
1	2.452749000	2.030401000	0.373545000
1	0.982126000	1.840214000	1.748147000
1	-1.019170000	1.084632000	1.345238000
1	1.390216000	0.367361000	0.475160000
6	0.529896000	-0.767108000	1.223176000
8	-0.686453000	-0.495386000	1.244691000
1	1.160478000	-0.637685000	2.114248000
1	0.916838000	-1.490055000	0.486484000

Mes'

E(RM062X) = -1205.15486266

7	-1.648260000	1.381204000	0.051382000
6	-1.109847000	2.406700000	-0.879352000
6	0.275153000	2.593651000	-0.918051000
5	1.401860000	1.888446000	0.033507000
6	2.668973000	1.404590000	-0.849431000
6	2.538657000	0.225785000	-1.599746000
6	3.884601000	2.106386000	-0.971261000
6	3.536868000	-0.287719000	-2.423891000
6	4.889650000	1.596014000	-1.800022000
6	4.747995000	0.414099000	-2.521484000
6	1.760678000	2.569853000	1.463707000
6	2.572562000	1.772164000	2.291844000
6	1.376063000	3.823119000	1.983299000
6	2.999402000	2.138786000	3.564491000
6	1.798450000	4.193992000	3.266475000
6	2.595782000	3.385085000	4.069215000
6	4.153475000	3.405733000	-0.243906000
1	4.992995000	3.934602000	-0.703482000
1	3.283689000	4.069667000	-0.257128000
1	4.392742000	3.235746000	0.810956000
6	5.863859000	-0.095161000	-3.396267000
1	6.194294000	-1.092408000	-3.084687000
1	5.547955000	-0.179247000	-4.442207000
1	6.727800000	0.572067000	-3.358390000
6	0.563531000	4.832772000	1.201313000
1	-0.405503000	4.442761000	0.873786000
1	0.378385000	5.722625000	1.808396000
1	1.085892000	5.150045000	0.293286000
6	3.024576000	3.837167000	5.440431000
1	2.682856000	3.143529000	6.216822000
1	4.115949000	3.889407000	5.521378000
1	2.622735000	4.826133000	5.671511000
6	-2.949368000	0.775104000	-0.334417000
1	-3.060898000	-0.129180000	0.263919000
1	-3.763529000	1.470939000	-0.131873000
1	-2.917719000	0.521568000	-1.393193000
6	-1.692338000	1.860019000	1.463613000
1	-2.424774000	2.666359000	1.532112000
1	-1.975747000	1.013213000	2.090588000
1	-0.701097000	2.220878000	1.743096000
6	0.711514000	3.532430000	-1.869354000
1	1.783024000	3.671535000	-1.989212000
6	-0.160871000	4.278089000	-2.652574000
1	0.229894000	4.998500000	-3.364233000
6	-2.015741000	3.141778000	-1.640869000
1	-3.084576000	2.974967000	-1.563605000
6	-1.535358000	4.097208000	-2.527669000
1	-2.229910000	4.674483000	-3.128200000
1	5.824449000	2.148203000	-1.887981000
1	1.497747000	5.167312000	3.651549000
1	2.917347000	0.815146000	1.896102000
6	3.876565000	1.225817000	4.381228000
1	3.397715000	0.948316000	5.327080000
1	4.101083000	0.307711000	3.834146000
1	4.827205000	1.706742000	4.636741000
1	1.595692000	-0.321340000	-1.543313000
6	3.323969000	-1.563877000	-3.196159000
1	2.330310000	-1.975089000	-3.004476000
1	3.419623000	-1.401497000	-4.275717000
1	4.062513000	-2.326638000	-2.924613000
8	-0.601428000	-0.931124000	0.679477000
6	0.526651000	-0.583061000	1.097498000
1	0.886229000	0.762003000	0.429347000
1	-1.015671000	0.545013000	0.076998000
1	0.647330000	-0.115705000	2.092784000
1	1.446916000	-1.044010000	0.699876000

Mes

E(RM062X) = -1205.14465089

7	-1.604437000	1.338153000	0.225233000
6	-1.105154000	2.361189000	-0.726003000
6	0.276048000	2.544848000	-0.848421000
5	1.496679000	1.838034000	-0.005465000
6	2.714660000	1.495954000	-1.026172000
6	2.542489000	0.490347000	-2.010673000
6	3.957020000	2.169875000	-1.007458000
6	3.601546000	0.111466000	-2.836360000
6	4.993846000	1.772068000	-1.858205000
6	4.849811000	0.723967000	-2.759595000
6	1.872414000	2.452395000	1.465978000
6	2.727350000	1.690192000	2.305581000
6	1.386468000	3.669887000	2.013013000
6	2.990681000	2.079240000	3.621306000
6	1.674857000	4.029484000	3.333554000
6	2.457614000	3.239783000	4.168450000
6	4.227718000	3.372596000	-0.125646000
1	4.461285000	3.095871000	0.907235000
1	5.075720000	3.938333000	-0.520950000
1	3.366223000	4.044358000	-0.078364000
6	5.995016000	0.272687000	-3.629052000
1	6.716934000	1.078693000	-3.783290000
1	6.530401000	-0.565615000	-3.170267000
1	5.642075000	-0.062143000	-4.608238000
6	0.597603000	4.692210000	1.217692000
1	-0.388587000	4.339537000	0.901341000

1	0.448821000	5.592757000	1.818372000
1	1.125189000	4.984680000	0.305997000
6	2.716357000	3.626037000	5.601525000
1	1.972544000	3.180019000	6.270699000
1	3.700393000	3.283738000	5.932091000
1	2.669376000	4.709948000	5.734036000
6	-2.905866000	0.712826000	-0.128001000
1	-2.987821000	-0.195760000	0.468621000
1	-3.727080000	1.392624000	0.099238000
1	-2.897196000	0.463425000	-1.188337000
6	-1.619342000	1.822485000	1.635075000
1	-2.335884000	2.642143000	1.715254000
1	-1.907100000	0.983601000	2.270472000
1	-0.617130000	2.164863000	1.898021000
6	0.650008000	3.498128000	-1.814288000
1	1.712278000	3.644514000	-1.992952000
6	-0.266099000	4.253514000	-2.535379000
1	0.083312000	4.982198000	-3.259974000
6	-2.052956000	3.109286000	-1.422298000
1	-3.115069000	2.944369000	-1.277629000
6	-1.630191000	4.072982000	-2.328568000
1	-2.360696000	4.656688000	-2.878064000
1	5.941042000	2.307743000	-1.817851000
1	1.283002000	4.969980000	3.716919000
8	-0.536943000	-0.939977000	0.757329000
6	0.650317000	-0.677234000	1.063033000
1	1.059281000	0.645702000	0.355471000
1	-0.966661000	0.497104000	0.249566000
1	0.904296000	-0.229082000	2.040539000
1	3.442364000	-0.673706000	-3.573799000
6	1.197473000	-0.151880000	-2.284331000
1	0.518834000	0.578791000	-2.740177000
1	1.307034000	-0.981197000	-2.987676000
1	0.692210000	-0.537188000	-1.396131000
6	3.499873000	0.476928000	1.825148000
1	4.514174000	0.777958000	1.535922000
1	3.594836000	-0.263327000	2.625496000
1	3.075870000	0.000727000	0.945551000
1	3.647378000	1.458491000	4.229506000
1	1.476563000	-1.223127000	0.578606000

FMes

E(RM062X) = -2991.59788324

7	-2.058873000	1.970327000	0.211979000
6	-1.269243000	2.708578000	-0.794639000
6	0.139578000	2.654507000	-0.853139000
5	1.265869000	1.845281000	0.062101000
6	2.490572000	1.351912000	-0.942144000
6	2.391407000	0.181476000	-1.738102000
6	3.708511000	2.051797000	-1.091935000
6	3.432877000	-0.292755000	-2.524793000
6	4.759742000	1.585386000	-1.886131000
6	4.631569000	0.402902000	-2.583970000
6	1.854997000	2.342070000	1.536390000
6	2.810089000	1.555403000	2.236294000
6	1.507703000	3.544067000	2.206421000
6	3.390893000	1.963017000	3.440889000
6	2.087029000	3.952090000	3.402653000
6	3.044456000	3.165407000	4.017574000
6	4.025397000	3.368759000	-0.406792000
6	5.734961000	-0.111595000	-3.462406000
6	0.431152000	4.478733000	1.702332000
6	3.709840000	3.640321000	5.276843000
6	-2.632000000	0.725679000	-0.364312000
1	-3.061178000	0.135776000	0.449916000
1	-3.411273000	0.979933000	-1.087802000
1	-1.847873000	0.166145000	-0.867885000
6	-3.156826000	2.751015000	0.845496000
1	-3.394049000	2.266680000	1.795783000
1	-2.825058000	3.768988000	1.024904000
1	-4.046434000	2.751406000	0.212326000
6	0.677884000	3.370914000	-1.943819000
1	1.750045000	3.377014000	-2.081452000
6	-0.070451000	4.096039000	-2.860118000
1	0.433141000	4.629974000	-3.659218000
6	-2.041324000	3.416898000	-1.717491000
1	-3.123140000	3.410759000	-1.626619000
6	-1.453376000	4.125205000	-2.751992000
1	-2.065131000	4.675399000	-3.458567000
1	5.678901000	2.154206000	-1.955614000
1	1.783424000	4.882057000	3.865321000
8	-0.783225000	1.038234000	2.113788000
6	-0.106852000	0.143351000	1.513158000
1	0.670524000	0.723642000	0.451410000
1	-1.422454000	1.608845000	1.143664000
1	0.746738000	-0.300311000	2.031933000
1	3.313623000	-1.206001000	-3.095625000
6	1.141245000	-0.668287000	-1.776575000
6	3.436606000	0.246273000	1.770305000
1	4.122357000	1.331526000	3.929284000
9	6.891427000	0.522058000	-3.235038000
9	5.438033000	0.046035000	-4.761363000
9	5.938314000	-1.422429000	-3.268685000
9	0.025868000	0.068875000	-1.928649000
9	0.965715000	-1.408950000	-0.666949000
9	1.157050000	-1.534096000	-2.799933000
9	4.599052000	3.205169000	0.793313000
9	2.947554000	4.145374000	-0.238811000
9	4.891652000	4.087844000	-1.142570000
9	0.654339000	4.974478000	0.485701000
9	0.261957000	5.539371000	2.509646000
9	-0.763278000	3.850945000	1.676685000
9	2.664181000	-0.526194000	0.994067000
9	3.754408000	-0.525946000	2.826368000
9	4.579627000	0.460195000	1.102245000
9	4.705837000	4.498007000	5.012891000
9	2.843949000	4.281514000	6.074914000
9	4.234634000	2.624002000	5.973822000
1	-0.591921000	-0.529338000	0.791596000

CF_3

E(RM062X) = -1181.39197276

7	-1.693634000	1.692376000	0.917036000
6	-1.096903000	2.386528000	-0.240930000
6	0.271501000	2.284493000	-0.518646000
5	1.366170000	1.620282000	0.440630000
6	-2.567643000	0.574038000	0.480108000
1	-2.870066000	0.014302000	1.366749000
1	-3.443187000	0.954798000	-0.049696000
1	-1.992159000	-0.071493000	-0.184830000
6	-2.417951000	2.605701000	1.837772000
1	-3.350651000	2.949421000	1.385743000
1	-2.632523000	2.050481000	2.753190000
1	-1.768575000	3.448001000	2.064347000
6	0.712650000	2.928680000	-1.687952000
1	1.765814000	2.881046000	-1.942358000
6	-0.146926000	3.638713000	-2.517394000
1	0.239670000	4.124074000	-3.407373000
6	-1.973548000	3.094132000	-1.061748000
1	-3.030854000	3.148044000	-0.818918000
6	-1.498764000	3.727220000	-2.202728000
1	-2.182410000	4.276717000	-2.840874000
1	-0.978187000	1.111962000	1.643179000
1	0.937040000	0.437539000	0.801523000

6	0.495992000	-0.338313000	1.845566000
8	-0.415961000	0.280919000	2.496556000
1	1.475824000	-0.483921000	2.315173000
6	1.607048000	2.466851000	1.796052000
9	2.367464000	3.553217000	1.545838000
9	0.452631000	2.944552000	2.339827000
9	2.225838000	1.784551000	2.780166000
6	2.756282000	1.176993000	-0.244630000
9	3.538973000	2.217400000	-0.613994000
9	3.505416000	0.416988000	0.586861000
9	2.567310000	0.437485000	-1.363411000
1	0.216370000	-1.142216000	1.141438000

PFtB

E(RM062X) = -2608.13979769

7	-1.159911000	0.367017000	-0.244820000
6	-0.998205000	1.809507000	-0.496023000
6	0.088942000	2.588106000	-0.035173000
5	1.559777000	2.171161000	0.602137000
6	2.846955000	2.422962000	-0.587626000
6	2.239829000	2.026542000	-1.962858000
6	4.103675000	1.519366000	-0.403721000
6	1.691509000	2.568502000	2.270133000
6	3.026248000	2.207959000	2.956811000
6	0.616758000	1.787058000	3.078571000
6	3.414128000	3.858659000	-0.757084000
9	4.187489000	4.191781000	0.274793000
9	4.163358000	3.952944000	-1.866107000
9	2.472275000	4.793930000	-0.881448000
6	1.453313000	4.065799000	2.562125000
9	1.863064000	4.431463000	3.779491000
9	2.116583000	4.839895000	1.692430000
9	0.153263000	4.368912000	2.479540000
9	4.755147000	1.763582000	0.724494000
9	5.008241000	1.653952000	-1.376996000
9	3.747182000	0.219628000	-0.400477000
9	3.140388000	1.794411000	-2.918473000
9	1.418146000	2.960172000	-2.436011000
9	1.534136000	0.878023000	-1.846530000
9	3.971029000	3.098174000	2.656971000
9	3.448282000	0.985668000	2.602060000
9	2.918736000	2.185981000	4.291836000
9	-0.525868000	1.623874000	2.400522000
9	0.298516000	2.404764000	4.220549000
9	1.062024000	0.569996000	3.404814000
1	-0.320818000	-0.278857000	0.583631000
1	1.656724000	0.843235000	0.714394000
6	-2.068557000	2.377431000	-1.193935000
1	-2.862778000	1.731750000	-1.555872000
6	-2.156789000	3.740105000	-1.420051000
1	-2.996081000	4.154587000	-1.968014000
6	-0.084850000	3.973147000	-0.236680000
1	0.665392000	4.652505000	0.127779000
6	-1.159120000	4.548824000	-0.899515000
1	-1.199094000	5.626869000	-1.013489000
6	1.528764000	-0.534533000	0.814821000
8	0.364643000	-0.817424000	1.285026000
6	-2.385023000	0.091485000	0.546546000
1	-3.291685000	0.268228000	-0.038703000
1	-2.359568000	-0.956694000	0.857525000
1	-2.387412000	0.727430000	1.429768000
6	-1.176406000	-0.449138000	-1.477630000
1	-0.330539000	-0.180441000	-2.105474000
1	-1.103909000	-1.502665000	-1.191520000
1	-2.103514000	-0.301741000	-2.041570000
1	1.711007000	-0.668151000	-0.254392000
1	2.384798000	-0.694380000	1.470599000

C_6F_5

E(RM062X) = -1961.68202993

7	-1.501602000	1.775881000	0.821038000
6	-1.107145000	2.367765000	-0.481126000
6	0.199988000	2.229263000	-0.972349000
5	1.448262000	1.518241000	-0.213913000
6	2.794993000	1.372298000	-1.092490000
6	3.205111000	0.173597000	-1.661591000
6	3.651318000	2.452184000	-1.280835000
6	4.392022000	0.038240000	-2.372227000
6	4.843126000	2.365410000	-1.987277000
6	5.215217000	1.143542000	-2.533535000
6	1.782744000	2.059630000	1.271354000
6	2.429794000	1.236680000	2.192315000
6	1.535392000	3.352313000	1.716966000
6	2.766167000	1.637580000	3.477298000
6	1.845599000	3.797178000	2.996505000
6	2.468988000	2.931980000	3.882670000
6	-2.680214000	0.870057000	0.713220000
1	-2.772328000	0.332383000	1.657247000
1	-3.583823000	1.444640000	0.510886000
1	-2.501064000	0.164957000	-0.097884000
6	-1.735405000	2.808807000	1.869662000
1	-1.744735000	2.313326000	2.842225000
1	-0.939215000	3.546821000	1.819033000
1	-2.695275000	3.295851000	1.686585000
6	0.417536000	2.822988000	-2.227494000
1	1.404416000	2.739020000	-2.670228000
6	-0.563778000	3.516862000	-2.925662000
1	-0.331462000	3.956818000	-3.889945000
6	-2.104753000	3.073065000	-1.150358000
1	-3.095516000	3.173136000	-0.716672000
6	-1.835453000	3.654225000	-2.381962000
1	-2.611587000	4.200656000	-2.906492000
8	-0.143101000	-0.178334000	1.750151000
6	0.310468000	-0.691452000	0.693330000
1	1.134556000	0.292007000	-0.021820000
1	-0.760307000	1.069987000	1.221943000
1	1.137013000	-1.410773000	0.739806000
9	4.744585000	-1.134030000	-2.898815000
9	6.352887000	1.035854000	-3.214642000
9	5.627599000	3.430160000	-2.148045000
9	3.315724000	3.650629000	-0.780868000
9	2.446048000	-0.928674000	-1.540674000
9	2.766826000	-0.011662000	1.845780000
9	0.930064000	4.245798000	0.913955000
9	1.547397000	5.041495000	3.373989000
9	2.778209000	3.337600000	5.110836000
9	3.375579000	0.804068000	4.318338000
1	-0.327387000	-0.788993000	-0.205321000

8. Substrates

H_2

E(RM062X) = -1.16799951607

1	-0.493945000	-0.039990000	-0.199304000
1	-0.841935000	0.039990000	-0.844352000

CO_2

E(RM062X) = -188.575018237

6	-0.667940000	0.000000000	-0.521828000
8	-0.119089000	-0.126145000	0.495542000
8	-1.216791000	0.126145000	-1.539198000

HCOOH (cis)

E(RM062X) = -189.747609439

1	-2.206003000	1.596537000	-2.587893000
8	-2.220377000	0.647685000	-2.762584000
8	-2.261354000	-1.227016000	-1.562310000
6	-2.242418000	-0.035246000	-1.604496000
1	-2.241376000	0.609967000	-0.706594000

HCOOH (trans)

E(RM062X) = -189.753310212

1	-2.247340000	-0.002391000	-3.489419000
8	-2.247340000	0.646784000	-2.768016000
8	-2.247340000	-1.242536000	-1.545859000
6	-2.247340000	-0.046002000	-1.622018000
1	-2.247340000	0.644145000	-0.767731000

$CH_2(OH)_2$

E(RM062X) = -190.941235443

8	-1.449236000	1.159035000	-0.717566000
6	-1.296536000	-0.087962000	-0.103906000
1	-0.389369000	-0.605658000	-0.436568000
1	-1.220102000	0.124185000	0.968813000
1	-1.481403000	1.007209000	-1.669899000
8	-2.348492000	-0.961445000	-0.396554000
1	-3.160309000	-0.548581000	-0.077919000

CH_2O

E(RM062X) = -114.489434265

8	-1.245434000	-0.000006000	-2.579812000
6	-1.245430000	-0.000001000	-1.378331000
1	-1.245428000	0.937884000	-0.790103000
1	-1.245428000	-0.937877000	-0.790090000

H2O

E(RM062X) = -76.4252795782

8	0.310597000	1.642578000	-0.417528000
1	0.310597000	2.402838000	0.171539000
1	0.310597000	0.882319000	0.171539000

CH_3OH

E(RM062X) = -115.707294519

6	-1.370669000	-0.000387000	-0.682198000
1	-1.370669000	-0.835276000	-1.384989000
1	-2.261599000	0.610038000	-0.879695000
1	-0.479738000	0.610038000	-0.879695000
8	-1.370669000	-0.554016000	0.615331000
1	-1.370669000	0.169604000	1.249173000