Table 1 Selected Distances, Angles, and Torsions for **2.1**

Bond	Distance (Å)	
	Experimental	Calculated
Re(1)-C(16)	1.89(1)	1.916
Re(1)-C(17)	1.934(8)	1.936
Re(1)-C(18)	1.90(1)	1.918
Re(1)-N(1)	2.162(6)	2.197
Re(1)-N(2)	2.236(9)	2.293
Re(1)-Cl(1)	2.496(2)	2.525
C(16)-O(1)	1.16(1)	1.15323
C(17)-O(2)	1.12(1)	1.15039
C(18)-O(3)	1.15(1)	1.15627
Angle	**Degrees (°)**	
	Experimental	Calculated
C(16)-Re(1)-C(17)	87.6(4)	86.877
C(16)-Re(1)-C(18)	88.3(4)	90.613
C(17)-Re(1)-C(18)	87.3(4)	89.557
C(16)-Re(1)-N(1)	96.4(3)	96.240
C(17)-Re(1)-N(1)	174.9(3)	175.600
C(18)-Re(1)-N(1)	95.9(3)	93.506
C(16)-Re(1)-N(2)	169.3(3)	170.368
C(17)-Re(1)-N(2)	101.1(3)	102.755
C(18)-Re(1)-N(2)	98.3(3)	89.415
N(2)-Re(1)-N(1)	74.5(3)	74.146
C(16)-Re(1)-Cl(1)	91.7(3)	91.453
C(17)-Re(1)-Cl(1)	91.7(3)	94.786
C(18)-Re(1)-Cl(1)	179.9(3)	175.286
N(1)-Re(1)-Cl(1)	84.0(2)	82.058
N(2)-Re(1)-Cl(1)	81.6(2)	87.840
O(1)-C(16)-Re(1)	179.6(9)	178.224
O(2)-C(17)-Re(1)	176.0(8)	176.907
O(3)-C(18)-Re(1)	177.3(9)	179.317
Torsion	**Degrees (°)**	
	Experimental	Calculated
N(1)-C(5)-C(6)-N(2)	16(1)	15
N(2)-C(10)-C(11)-N(3)	41(1)	139

Table 2 Selected Distances, Angles, and Torsions for **2.2**

Bond	Distance (Å)	
	Experimental	Calculated
Re(1)-C(16)	1.926(9)	1.92438
Re(1)-C(17)	1.975(10)	1.90687
Re(1)-N(1)	2.119(7)	2.13186
Re(1)-N(2)	2.080(7)	2.08705
Re(1)-N(3)	2.126(7)	2.13185
Re(1)-Cl(1)	2.489(3)	2.53337
N(1)-N(3)	4.14(1)	4.14772
C(16)-O(1)	1.14(1)	1.16042
C(17)-O(2)	1.05(1)	1.16341
Angle	Degrees (°)	
	Experimental	Calculated
C(16)-Re(1)-C(17)	91.5(4)	89.188
C(16)-Re(1)-N(2)	173.7(4)	172.050
C(17)-Re(1)-N(2)	94.6(3)	98.762
C(16)-Re(1)-N(1)	103.9(3)	102.980
C(17)-Re(1)-N(1)	92.7(3)	93.429
N(2)-Re(1)-N(1)	77.3(3)	76.684
C(16)-Re(1)-N(3)	101.8(3)	102.986
C(17)-Re(1)-N(3)	91.7(3)	93.419
N(2)-Re(1)-N(3)	76.6(3)	76.684
N(1)-Re(1)-N(3)	153.7(3)	153.210
C(16)-Re(1)-Cl(1)	91.8(3)	89.136
C(17)-Re(1)-Cl(1)	176.5(2)	178.324
N(2)-Re(1)-Cl(1)	82.1(2)	82.913
N(1)-Re(1)-Cl(1)	85.4(2)	86.953
N(3)-Re(1)-Cl(1)	88.7(2)	86.953
O(1)-C(16)-Re(1)	177.9(9)	179.079
O(2)-C(17)-Re(1)	173.2(8)	179.182
Selected Torsions (deg)		
N(1)-C(5)-C(6)-N(2)	1(1)	2
N(2)-C(10)-C(11)-N(3)	-4(1)	-2

Table 3 Selected Distances, Angles, and Torsions for **2.3**

Bond	Distance (Å)	
	Experimental	Calculated
Re(1)-C(16)	1.911(3)	1.91740
Re(1)-C(17)	1.890(3)	1.91814
Re(1)-C(18)	1.921(4)	1.93897
Re(1)-N(1)	2.173(3)	2.19687
Re(1)-N(2)	2.232(2)	2.28998
Re(1)-Br(1)	2.6410(4)	2.67953
C(16)-O(1)	1.150(4)	1.15290
C(17)-O(2)	1.157(4)	1.15012
C(18)-O(3)	1.155(5)	1.15591
Angle	Degrees (°)	
	Experimental	Calculated
C(16)-Re(1)-C(17)	89.1(1)	90.772
C(16)-Re(1)-C(18)	85.9(1)	86.823
C(16)-Re(1)-N(1)	97.9(1)	96.034
C(17)-Re(1)-N(1)	92.5(1)	93.597
C(18)-Re(1)-N(1)	175.4(1)	175.575
C(16)-Re(1)-N(2)	171.2(1)	170.290
C(17)-Re(1)-N(2)	96.0(1)	89.435
C(18)-Re(1)-N(2)	101.3(1)	102.886
N(1)-Re(1)-N(2)	74.7(1)	74.265
C(16)-Re(1)-Br(1)	92.7(1)	90.399
C(17)-Re(1)-Br(1)	177.6(1)	176.076
C(18)-Re(1)-Br(1)	91.6(1)	94.069
N(1)-Re(1)-Br(1)	85.74(7)	82.555
N(2)-Re(1)-Br(1)	82.07(7)	88.780
O(1)-C(16)-Re(1)	178.6(3)	178.270
O(2)-C(17)-Re(1)	179.5(3)	179.355
O(3)-C(18)-Re(1)	179.9(3)	176.781
Selected Torsions (deg)		
N(1)-C(6)-C(1)-N(2)	-15.4(4)	-14.749
N(2)-C(5)-C(11)-N(3)	141.1(3)	136.119

Table 4 Selected Distances, Angles, and Torsions for **2.5**

Axial CN			Planar CN		
Bond	Distance (Å)		Bond	Distance (Å)	
	Exp.	Calc.		Exp.	Calc.
Re(2)-C(35)	2.148(7)	2.13963	Re(1)-C(19)	2.105(8)	1.98769
Re(2)-C(36)	1.926(6)	1.94011	Re(1)-C(16)	1.928(5)	2.09197
Re(2)-C(37)	1.954(7)	1.96758	Re(1)-C(18)	1.96(1)	2.00792
Re(2)-C(38)	1.902(9)	1.91853	Re(1)-C(17)	1.918(7)	1.90499
Re(2)-N(5)	2.242(7)	2.28998	Re(1)-N(1)	2.253(5)	2.32197
Re(2)-N(6)	2.168(5)	2.20279	Re(1)-N(2)	2.176(4)	2.18806
C(35)-N(8)	1.138(9)	1.16104	C(19)-O(3)	1.17(1)	1.14703
C(36)-O(4)	1.145(8)	1.15044	C(16)-N(4)	1.149(7)	1.16100
C(37)-O(5)	1.151(9)	1.15134	C(18)-O(2)	1.14(1)	1.14276
C(38)-O(6)	1.17(1)	1.15368	C(17)-O(1)	1.130(8)	1.15781
Angle	Degrees (°)		Angle	Degrees (°)	
	Exp.	Calc.		Exp.	Calc.
C(36)-Re(2)-C(38)	87.7(3)	87.273	C(16)-Re(1)-C(17)	87.8(3)	90.158
C(36)-Re(2)-C(37)	88.0(3)	89.890	C(16)-Re(1)-C(18)	87.0(3)	84.822
C(36)-Re(2)-C(35)	92.1(3)	93.356	C(16)-Re(1)-C(19)	92.5(3)	88.356
C(38)-Re(2)-C(37)	88.5(3)	90.973	C(17)-Re(1)-C(18)	88.7(3)	88.453
C(38)-Re(2)-C(35)	90.8(3)	91.628	C(17)-Re(1)-C(19)	90.5(3)	87.745
C(37)-Re(2)-C(35)	179.2(3)	175.933	C(18)-Re(1)-C(19)	179.1(3)	172.179
C(36)-Re(2)-N(5)	100.6(3)	102.576	C(16)-Re(1)-N(1)	102.2(2)	98.105
C(36)-Re(2)-N(6)	174.2(3)	175.708	C(16)-Re(1)-N(2)	175.9(2)	172.047
C(38)-Re(2)-N(5)	169.3(3)	170.146	C(17)-Re(1)-N(1)	168.3(3)	170.509
C(38)-Re(2)-N(6)	96.6(3)	96.171	C(17)-Re(1)-N(2)	95.9(3)	97.544
C(37)-Re(2)-N(5)	98.4(2)	89.360	C(18)-Re(1)-N(1)	97.7(3)	88.487
C(37)-Re(2)-N(6)	96.0(2)	92.605	C(18)-Re(1)-N(2)	94.8(3)	93.374
C(35)-Re(2)-N(5)	82.3(2)	87.543	C(19)-Re(1)-N(1)	83.2(2)	96.317
C(35)-Re(2)-N(6)	83.9(2)	84.008	C(19)-Re(1)-N(2)	85.7(2)	93.899
N(5)-Re(2)-N(6)	74.7(2)	73.977	N(1)-Re(1)-N(2)	73.9(2)	73.675
O(6)-C(38)-Re(2)	179.4(7)	178.027	O(1)-C(17)-Re(1)	178.2(7)	177.623
O(5)-C(37)-Re(2)	175.5(6)	179.414	O(2)-C(18)-Re(1)	172.0(7)	176.452
N(8)-C(35)-Re(2)	178.0(6)	176.457	O(3)-C(19)-Re(1)	178.0(6)	176.552
O(4)-C(36)-Re(2)	179.0(7)	177.313	N(4)-C(16)-Re(1)	178.7(6)	178.113
Torsion	Degrees (°)		Torsion	Degrees (°)	
	Exp.	Calc.		Exp.	Calc.
N(5)-C(20)-C(25)-N(6)	14.5(9)	13.735	N(1)-C(1)-C(6)-N(2)	12.5(8)	14.777
N(5)-C(24)-C(30)-N(7)	41(1)	135.774	N(1)-C(5)-C(11)-N(3)	43.7(9)	137.014

Table 5 Selected Distances, Angles and Torsions for Acetonitrile Adduct of **2.8**

Bond	Distance (Å)	
	Experimental	Calculated
Re(1)-C(16)	1.889(4)	1.93046
Re(1)-C(17)	1.885(3)	1.92844
Re(1)-N(1)	2.091(3)	2.10116
Re(1)-N(2)	2.135(3)	2.15397
Re(1)-N(3)	2.131(3)	2.15392
Re(1)-N(4)	2.160(3)	2.15202
N(2)-N(3)	4.138(4)	4.18483
C(16)-O(1)	1.170(4)	1.15749
C(17)-O(2)	1.171(4)	1.15244
Angle	Degrees (°)	
	Experimental	Calculated
C(16)-Re(1)-C(17)	87.69(16)	88.104
C(16)-Re(1)-N(1)	175.95(12)	176.094
C(17)-Re(1)-N(1)	96.35(12)	95.802
C(16)-Re(1)-N(3)	103.81(13)	103.594
C(17)-Re(1)-N(3)	94.03(12)	92.309
N(1)-Re(1)-N(3)	76.20(10)	76.306
C(16)-Re(1)-N(2)	103.58(13)	103.598
C(17)-Re(1)-N(2)	93.73(12)	92.307
N(1)-Re(1)-N(2)	75.99(10)	76.305
N(3)-Re(1)-N(2)	151.77(11)	152.544
C(16)-Re(1)-N(4)	90.50(14)	88.484
C(17)-Re(1)-N(4)	178.10(12)	176.587
N(1)-Re(1)-N(4)	85.46(10)	87.611
N(3)-Re(1)-N(4)	86.94(10)	88.504
N(2)-Re(1)-N(4)	86.15(10)	88.485
O(1)-C(16)-Re(1)	179.1(3)	178.807
O(2)-C(17)-Re(1)	178.0(3)	178.860
Torsion	Degrees (°)	
	Experimental	Calculated
N(1)-C(1)-C(6)-N(2)	1.7(4)	1.105
N(1)-C(5)-C(11)-N(3)	-1.8(4)	-1.110

Table 6 Selected Distances, Angles, and Torsions for κ^2(terpy)Mn(CO)$_3$Br from Compain et. al.

Selected Distances (Å)	
Mn(1)-N(1)	2.045(1)
Mn(1)-N(2)	2.105(2)
N(1)-N(2)	2.636(2)
Selected Angles (deg)	
N(1)-Mn(1)-N(2)	78.84(6)
Selected Torsions (deg)	
N(1)-C(8)-C(9)-N(2)	-16.5(2)
N(2)-C(13)-C(14)-N(3)	143.2(2)

Table 7 Crystal data and structure refinement for compounds **1**, **3**, **5**, and **7**

Compound	**1**	**3**	**5**	**7**
Empirical formula	$C_{19}H_{11}N_3O_3ReCl$	$C_{19}H_{11}N_3O_3ReBr$	$C_{20}H_{11}N_4O_3Re$	$C_{22}H_{14}N_4O_6F_3SRe$
Formula weight (g/mol)	538.96	583.41	530.04	693.63
Temperature (K)	200(2)	200	200	200
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
Crystal System	Triclinic	Monoclinic	Triclinic	
Space Group	P-1	C2/c	P-1	
a (Å)	9.8736(4)	31.1537(7)	9.9196(9)	
b (Å)	14.8202(4)	7.1176(2)	14.9902(14)	
c (Å)	16.3472(4)	16.8519(4)	16.5187(15)	
α (deg)	69.2890(10)	90.000	68.363(2)	
β (deg)	80.801(2)	111.0230(10)	80.929(2)	
γ (deg)	79.836(2)	90.000	79.975(2)	
Volume ($Å^3$)	2190.00(12)	3488.00	2236.6(4)	
Z, r (calc) (Mg/m^3)	2, 1.997	8, 2.222	2, 1.927	
Absorption coefficient (mm^{-1})	6.063	9.282	5.821	
Absorption correction		Semi-empirical from equivalents		
Final R indices [I≥2σ(I)]	R1 = 0.0397, wR2 = 0.0839	R1 = 0.0232, wR2 = 0.0614	R1 = 0.0390, wR2 = 0.0921	
R indices (all data)	R1 = 0.0604, wR2 = 0.0951	R1 = 0.0285, wR2 = 0.0642	R1 = 0.0500, wR2 = 0.0961	

Table 8 Crystal data and structure refinement for compounds **2**, **4**, **6**, and **8**

Compound	**2**	**4**	**6**	**8**
Empirical formula	$C_{18}H_{11}N_3O_2ReCl$	$C_{18}H_{11}N_3O_2ReBr$	$C_{19}H_{11}N_4O_2Re$	$C_{21}H_{14}N_4O_5F_3SRe$
Formula weight (g/mol)	510.95	530.04	502.04	665.61
Temperature (K)	200(2)	200	200	200
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
Crystal System	Triclinic			Triclinic
Space Group	P-1			P-1
a (Å)	8.5275(3)			8.5745(4)
b (Å)	14.2421(5)			11.9805(5)
c (Å)	17.4637(6)			13.0970(5)
α (deg)	77.948(2)			79.748(2)
β (deg)	85.684(2)			81.106(2)
γ (deg)	79.890			88.091(2)
Volume ($Å^3$)	2041.79(12)			1307.99(10)
Z, r (calc) (Mg/m^3)	4, 2.050			2, 1.993
Absorption coefficient (mm^{-1})	6.494			5.094
Absorption correction		Semi-empirical from equivalents		
Final R indices [I≥2σ(I)]	R1 = 0.0636, wR2 = 0.1018			R1 = 0.0294, wR2 = 0.0673
R indices (all data)	R1 = 0.0985, wR2 = 0.1110			R1 = 0.0366, wR2 = 0.0700

Table 9 Solvated and Gas Phase Energies of Axial & Trans $\kappa^{x}-(terpy)-Re(CO)_{5-x}CN$ (x=2,3)

Geometry	Bidentate		Terdentate	
	E(gas)[a]	E(solution)[b]	E(gas)[a]	E(solution)[b]
Axial	-1254.96132	-1254.99059	-1141.57255	-1141.60827
Trans	-1254.93788	-1254.97168	-1141.54660	-1141.58209
Difference	0.02343	0.01891	0.02595	0.02612
Difference (kcal/mol)	14.70	11.87	16.28	16.43

[a] B3LYP SCF energy in hartrees.
[b] B3LYP SCF energy in hartrees with PCM solvation in acetonitrile.

Table 10 Gas phase and solvated energies of compounds, transition states and intermediates in the 'carbonate' mechanism

Molecule	Label	E (gas)[a]	E (solution)[b]	E (solvation)[c]
Catalyst - CO_2	**4.11**	-1103.009	-1103.016	4.47
CO_2 Linked Dimer	**4.12**	-2017.373	-2017.412	24.59
CO_2 Addition TS	**4.13**	-2206.121	-2206.165	27.80
C_2O_4 Linked Dimer	**4.14**	-2206.048	-2206.097	31.23
5 Member Ringed Dimer TS	**4.15**	-2206.014	-2206.062	29.87
CO_3 Linked Dimer	**4.16**	-2092.678	-2092.726	29.75
Bicarbonate Catalyst Cation	**4.17**	-1178.065	-1178.120	34.24
Bicarbonate Anion	**4.18**	-264.485	-264.497	7.20
Open Site Cation	**4.19**	-914.106	-914.187	50.75

[a] TPSS SCF energy in hartrees. [b] TPSS SCF energy in hartrees with COSMO solvation in DMF. [c] TPSS solvation energy in kcal/mol (E(gas) - E(solution)).

Table 11 Energies for the reaction steps in the 'carbonate' pathway

Steps	Energy(gas)[a]	Energy(dmf)[b]
4.03 + **4.09** → **4.11**	-0.25	6.37
4.11 + **4.03** → **4.12**	-31.56	-42.39
4.12 + **4.09** → **4.13**	-33.27	-34.66
4.13 → **4.14**	45.91	42.47
4.14 → **4.15**	21.10	22.46
4.15 → **4.16** + **4.10**	-24.36	-24.84
4.16 → **4.17** + **4.19**	317.95	262.71
4.17 + **4.19** + **4.04**(x 2) → **4.01**(x 2) + **4.18**	-180.55	-239.63

[a] TPSS SCF energy in kcal/mol.
[b] TPSS SCF energy in kcal/mol with COSMO solvation in DMF.

Table 12 Gas phase and solvated energies of compounds, transition states and intermediates in the 'formate' mechanism

Molecule	Label	E (gas)[a]	E (solution)[b]	E (solvation)[c]
Proton Transfer TS	**4.21**	-1206.302	-1206.327	15.10
Catalyst Hydride	**4.22**	-914.920	-914.945	15.29
CO_2 Insertion TS	**4.23**	-1103.581	-1103.620	24.32
Catalyst Formate	**4.24**	-1103.635	-1103.665	19.04
Formate Anion	**4.25**	-189.305	-189.415	69.01
Open Site Cation	**4.27**	-914.106	-914.187	50.75

[a] TPSS SCF energy in hartrees.
[b] TPSS SCF energy in hartrees with COSMO solvation in DMF.
[c] TPSS solvation energy in kcal/mol (E(gas) - E(solution)).

Table 13 Energies for the reaction steps in the 'formate' pathway

Steps	Energy(gas)[a]	Energy(dmf)[b]
4.03 + **4.07** → **4.21**	-44.98	-48.46
4.21 → **4.22** + **4.26**	22.43	18.60
4.22 + **4.09** → **4.23**	21.24	14.02
4.23 → **4.24**	-33.94	-28.66
4.24 → **4.25** + **4.27**	140.39	39.67
4.27 + **4.04** → **4.01**	-141.77	-36.37

[a] TPSS SCF energy in kcal/mol.
[b] TPSS SCF energy in kcal/mol with COSMO solvation in DMF.

Table 14 Energies for the reaction steps in the 'equatorial' geometry

Steps	Energy(gas)[a]	Energy(dmf)[b]
4.03 → **4.34**	23.37	19.77
4.34 + **4.09** → **4.35**	4.79	1.56
4.35 + **4.07** → **4.36**	-36.36	-49.13
4.36 → **4.37** + **4.26**	-3.39	8.34
4.37 → **4.38** + **4.39**	-14.52	-0.35
4.38 → **4.27** + **4.10**	40.89	35.57
4.27 + **4.04** → **4.01**	-141.77	-36.37

[a] TPSS SCF energy in kcal/mol.
[b] TPSS SCF energy in kcal/mol with COSMO solvation in DMF.

Table 15 Gas phase and solvated energies of mechanism reactants and products.

Molecule	Label	E (gas)[a]	E (solution)[b]	E (solvation)[c]
Ground State	**4.01**	-1374.621419	-1374.651099	18.62
3MLCT Complex	**4.01$^{\mathbf{3MLCT}}$**	-1374.553193	-1374.565998	8.04
Radical Anion	**4.02**	-1374.684002	-1374.759190	47.18
Open Site Excimer	**4.03**	-914.3139376	-914.3287245	9.28
Chlorine Anion	**4.04**	-460.2890817	-460.4058583	73.28
Triethylamine (TEA)	**4.05**	-292.3051496	-292.3854033	50.36
Radical Cation TEA	**4.06**	-292.3051496	-292.3854033	50.36
Deprotonated TEA Radical	**4.07**	-291.9173706	-291.9211226	2.35
Triethylammonia	**4.08**	-292.9552538	-293.0382729	52.09
Carbon Dioxide	**4.09**	-188.6945676	-188.6974631	1.82
Carbon Monoxide	**4.10**	-113.3744946	-113.3754466	0.60
Diethylaminoethene	**4.26**	-291.3467768	-291.3525868	3.64

[a] TPSS SCF energy in hartrees. [b] TPSS SCF energy in hartrees with COSMO solvation in DMF. [c] TPSS solvation energy in kcal/mol (E(gas) - E(solution)).

Table 16 Energies for the reaction steps in the excimer formation pathway

Steps	Energy(gas)[a]	Energy(dmf)[b]
4.01 $\rightarrow$ **4.01**$^{\mathbf{3MLCT}}$	42.81	53.40
4.01$^{\mathbf{3MLCT}}$ + **4.05** $\rightarrow$ **4.02** + **4.06**	81.45	-5.80
4.02 $\rightarrow$ **4.03** + **4.04**	50.82	15.44
4.06 + **4.05** $\rightarrow$ **4.07** + **4.08**	-1.08	-2.92

[a] TPSS SCF energy in kcal/mol. [b] TPSS SCF energy in kcal/mol with COSMO solvation in DMF.

Table 17 Gas phase and solvated energies of compounds, transition states and intermediates in the 'water-gas shift' mechanism

Molecule	Label	E (gas)[a]	E (solution)[b]	E (solvation)[c]
Catalyst-CO_2 (Axial)	**4.31**	-1103.009	-1103.016	4.47
H Transfer to Axial CO_2 TS	**4.32**	-1394.981	-1395.011	18.86
Catalyst-CO_2H (Axial)	**4.33**	-1103.610	-1103.640	18.90
Catalyst with Migrated Open Site	**4.34**	-914.277	-914.297	12.88
Catalyst-CO_2 (Equatorial)	**4.35**	-1102.964	-1102.992	17.92
H Transfer to Equatorial CO_2 TS	**4.36**	-1394.939	-1394.992	33.05
Catalyst-CO_2H (Equatorial)	**4.37**	-1103.597	-1103.626	17.68
Tetracarbonyl Catalyst Cation	**4.38**	-1027.546	-1027.619	46.02
Water	**4.39**	-76.464	-76.476	7.33

[a] TPSS SCF energy in hartrees.
[b] TPSS SCF energy in hartrees with COSMO solvation in DMF. [c] TPSS solvation energy in kcal/mol (E(gas) - E(solution)).

Table 18 Energies for the reaction steps in the 'water-gas shift' mechanism

Steps	Energy(gas)[a]	Energy(dmf)[b]
4.03 + **4.09** → **4.31**	-0.25	6.37
4.31 + **4.07** → **4.32**	-34.68	-46.72
4.32 → **4.33** + **4.26**	15.33	11.64
4.33 → **4.38** + **4.39**	-6.51	8.88
4.38 → **4.27** + **4.10**	40.89	35.57
4.27 + **4.04** → **4.01**	-141.77	-36.37

[a] TPSS SCF energy in kcal/mol.
[b] TPSS SCF energy in kcal/mol with COSMO solvation in DMF.