

Supplimentary Information for
Switching of Reaction Enthalpy from Exothermic to Endothermic for
Decomposition of H₂CO₃ under Confinement

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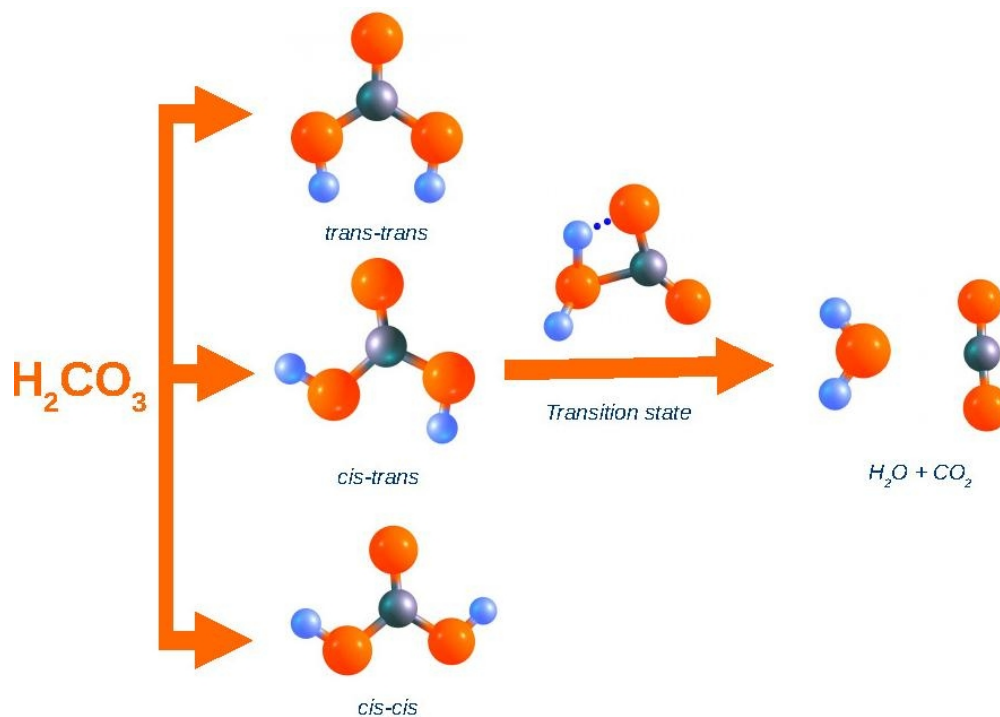
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Figure S1: The geometries and structures of all the isomers of Carbonic acids.**Table S1:** Comparison of the reaction energetics for the decomposition reaction of carbonic acid in gas phase.

Level of calculations	Energy Barrier (kcal mol^{-1})	Reaction energy (kcal mol^{-1})
CCSD(T)/cc-pVQZ//MP2/aug-cc-pVTZ ¹	40.9	-8.6
QCISD(T)/6-31 1++G** ²	41.4	-10.1
CCSD(T)/aug-cc-pVTZ//MP2/aug-cc-pVTZ ³	39.9	-10.7
DLPNO-CCSD(T)/cc-pVTZ//M06-2X/6-31G** ⁴	40.7	-9.3

1. Wagner, J. P., Reisenauer, H. P., Hirvonen, V., Wu, C. H., Tyberg, J. L., Allen, W. D., & Schreiner, P. R. Tunnelling in carbonic acid. *Chem. Commun.*, 52(50), 2016 7858-7861.

- Wight, C. A., & Boldyrev, A. I. Potential energy surface and vibrational frequencies of carbonic acid. *J. Phys. Chem.* , 99(32), **1995**, 12125-12130.
- Bandyopadhyay, B., Biswas, P., & Kumar, P. . Ammonia as an efficient catalyst for decomposition of carbonic acid: a quantum chemical investigation. *Phys. Chem. Chem. Phys.*, 18(23), **2016**, 15995-16004.
- Present work.

Table S2: Cartesian coordinates and normal mode frequencies obtained at M06-2X/6-31G** level:

Species	Cartesian Coordinates				Frequencies
CA					493.7501
					552.0407
					580.4767
	C	-0.05676500	-0.13362000	-0.00006200	616.9107
	O	-0.76688900	-1.09590700	0.00002400	792.9607
	O	1.27588900	-0.18033800	0.00001700	1017.1099
	H	1.62666400	0.71995600	0.00001300	1190.0902
O	-0.48797200	1.14710300	-0.00000100	1280.0534	
H	-1.45429600	1.11489500	0.00003500	1463.4004	
				1976.1589	
				3873.5923	
				3874.6811	
TS	C	0.33172900	0.09416900	-0.01166100	-1681.8080
	O	1.35636000	-0.48104500	0.00080600	425.9469
	O	-0.21745300	1.22591400	0.02563500	523.4253
	H	-1.23251200	0.47155500	0.03934500	623.1467
	O	-1.08119500	-0.70943200	-0.10216700	794.7900
	H	-1.21955300	-1.32006100	0.63642600	809.8179
				965.8993	
				1309.7105	

					1345.9472 2076.6465 2253.0411 3855.4323
CW	C	0.82312600	-0.00038900	0.00129700	90.7296
	O	0.85679300	1.16242700	0.00561700	164.2839
	O	0.85389000	-1.16331500	0.00558600	202.1752
	H	-2.22270400	-0.76591300	0.28251000	224.7235
	O	-1.77200400	0.00113500	-0.08287100	285.0313
	H	-2.22548600	0.76626600	0.28304400	648.0541
					674.1657
					1419.0464
					1641.7909
					2489.7651
					3888.8463
					4009.9766
CO ₂	C	0.00000000	0.00000000	0.00000100	668.2943
	O	0.00000000	0.00000000	-1.16279200	668.2943
	O	0.00000000	0.00000000	1.16279200	1421.6361
					2492.2642
H ₂ O	H	0.76025000	-0.47119700	0.00000000	1647.4744
	O	0.00000000	0.11779900	0.00000000	3884.0081
	H	-0.76025000	-0.47119700	0.00000000	4000.8925
C60	C	-0.37074000	-2.06297800	-2.85172800	267.9640
	C	0.08809300	-0.81892000	-3.44190200	268.0433
	C	1.39027800	-0.39000500	-3.23132700	268.1336
	C	2.29413400	-1.18531800	-2.42060300	268.1875
	C	1.85557600	-2.37418200	-1.85643600	268.4123
	C	0.49297500	-2.82295700	-2.07690800	343.5538
	C	-1.74919300	-1.88042800	-2.43533900	343.9544
	C	-2.14232100	-0.52347000	-2.76817000	344.2744
	C	-1.00676200	0.13246700	-3.39021200	360.8684
	C	-0.75088200	1.47065100	-3.13038600	361.0736
	C	1.65798900	1.01029500	-2.95915000	361.2257
	C	3.12037100	-0.27639500	-1.64729600	361.8077
	C	3.47172000	-0.59680200	-0.34421800	409.7212
	C	3.01283300	-1.84096700	0.24607300	409.8624
	C	2.22308500	-2.70940500	-0.49288700	410.0426
	C	1.08772500	-3.36557800	0.12931100	410.0577
	C	0.01844800	-3.43577300	-0.84973700	410.2300
	C	-1.29882300	-3.26130200	-0.45174100	441.3583
	C	-2.20267800	-2.46599200	-1.26254900	441.4536
	C	-2.97148100	0.18789200	-1.91356200	441.7074
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	C	-2.70275500	-2.05692300	0.99525100	495.3983
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C	2.72726000	1.08052300	-1.98018000	544.7818
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C	2.14232000	0.52346500	2.76817200	564.7501
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C	-1.08772700	3.36558000	-0.12930900	582.0148
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	C	0.48175600	0.35124000	3.43347100	86.6201
	C	-0.08232400	1.64106600	3.08815400	125.2758
	C	-1.41608700	1.75318300	2.71493800	220.8528
	C	-2.23195300	0.55225400	2.65467900	275.6687
	C	-2.04199200	-1.88462100	2.23261200	281.8812

C	-0.83532400	-2.71109500	2.14948400	291.5745
C	0.23511600	-2.02052200	2.86536700	295.1461
C	1.54849700	-2.04641900	2.40029500	302.6704
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C	0.94098300	2.39792600	2.39556200	309.7568
C	0.57176500	3.23239200	1.35176200	364.4563
C	-0.83341800	3.37916500	0.95944000	372.4970
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C	3.19654900	-0.66472900	-1.54616700	526.9261
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C	0.30914700	0.78176500	-3.38157100	543.4354
C	-0.23507600	2.02112600	-2.85878300	555.6072
C	0.82525300	2.68662900	-2.12676700	557.2186
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C	1.40532200	3.24218600	0.16503900	560.5304
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C	3.57206600	0.37623000	0.67396800	563.5060
C	3.27572400	-0.84502900	1.29751900	563.8515
C	2.93147000	-2.02643400	0.49977400	567.5864
C	2.89114800	-1.93729900	-0.88576300	571.2661
C	1.79353700	-2.58394900	-1.60397500	572.5015
C	1.41753700	-1.72437300	-2.70245100	572.8951
C	0.08397000	-1.64334200	-3.08762300	573.2226
C	-0.47961400	-0.35476800	-3.43448100	577.8611
C	-1.55138500	2.08493300	-2.41459800	581.4792
C	-2.36393500	0.87750900	-2.45727500	590.3011
C	-1.84810600	-0.31250000	-2.96004600	592.6352
C	-2.14525400	-1.59311000	-2.33300200	595.4280
C	-0.94592300	-2.41848600	-2.41445300	598.5613
C	-0.59885800	-3.26315800	-1.36555000	603.2299
C	0.80274900	-3.32127400	-0.95270600	606.3752
C	0.84364600	-3.41598900	0.49019500	612.7550
C	1.86730900	-2.76211400	1.18370500	636.3242

C	2.97000700	1.60998200	1.20129600	669.1989
C	2.39845800	-0.86468300	2.46506000	673.5643
C	1.70506500	0.68697800	-2.98607500	673.7370
C	0.17666900	0.14139800	-0.03606400	680.2736
O	1.33251600	-0.05426800	-0.00235600	681.0012
O	-0.62756400	1.08071600	-0.00086500	683.0474
H	-1.38623700	-0.04472800	0.08657300	731.2880
O	-0.71455000	-0.95459100	-0.07094800	732.7538
H	-0.51293000	-1.58360700	0.65408500	735.1202
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		978.0883 983.5713 990.2373 990.9698 1036.9035 1061.6297 1071.0486 1074.7123 1092.4420 1127.1055 1128.3743 1130.6849 1131.0561 1132.0646 1164.4418 1171.0421 1177.4546 1203.1383 1210.6727 1225.5915 1234.1614 1237.0472 1242.4226 1255.2661 1257.1453 1259.4068 1269.6803 1279.1046 1283.2712 1288.6287 1291.2204 1291.4515 1303.6098 1304.5765 1307.7812 1324.5715 1328.5890 1330.3339 1332.5239 1333.8141 1336.4715 1338.7896 1343.8552 1373.9630 1379.4665 1381.5641 1385.1479 1386.1479 1390.4517 1394.9432
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					1396.5826 1419.3569 1431.3985 1444.3819 1453.5497 1456.3882 1462.1730 1464.5033 1467.0244 1467.9733 1474.5676 1486.3695 1497.1091 1508.2308 1519.2849 1547.6670 1549.6564 1555.3039 1560.9866 1573.8618 1580.5206 1587.0307 1620.4782 1624.4408 1627.6182 1633.6738 1635.1654 1638.4506 1646.4801 1648.2181 1654.9351 1658.0718 2149.3737 2373.1235 3461.6070
CW@C60	C	1.67863700	1.82068500	2.50869800	54.1663
	C	0.29123400	1.87060800	2.95203600	65.6009
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	C	0.40698600	-0.54003300	3.41787800	222.0983
	C	1.73032900	-0.58433000	3.00109000	273.5902
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	C	1.81184600	2.72290700	1.37574700	291.6481
	C	0.49430800	3.32663200	1.13916800	297.0908
	C	-0.44349100	2.80858700	2.12100500	298.2256
	C	-1.77470500	2.56320400	1.77501300	304.7484
	C	-1.69870400	0.43509300	3.03350200	305.1951
	C	-0.51504100	-1.60466000	3.07302000	364.0350
	C	-0.09311600	-2.68962800	2.31493300	375.8165
	C	1.28589100	-2.72030800	1.85517300	377.9889

C	2.18149600	-1.70079800	2.19794700	387.9263
C	3.15072400	-1.17857800	1.23366000	391.4666
C	3.30528500	0.27049100	1.44772200	405.9618
C	3.45492100	1.13844200	0.35021600	407.0499
C	2.68139800	2.39735800	0.32261100	407.0742
C	0.05433600	3.56260100	-0.15408300	407.7919
C	0.92722500	3.16864000	-1.25278500	408.5795
C	2.20258900	2.61907900	-1.03975800	409.1166
C	2.67472000	1.50732600	-1.85541000	422.9356
C	3.44308600	0.58392300	-1.01306500	458.4791
C	3.29278500	-0.80179100	-1.20650300	462.7038
C	3.14147500	-1.70232700	-0.06203500	468.4804
C	2.18843100	-2.76657200	-0.41163300	469.1794
C	1.29132100	-3.29069500	0.51980700	471.7424
C	-1.81280200	-1.00003300	2.83380800	501.4884
C	-1.83182900	-2.77615500	-1.39515800	509.1557
C	-2.65233700	-2.41429800	-0.32751800	515.7438
C	-3.34734200	-1.12108300	-0.34622600	520.5787
C	-3.23368300	-0.24473100	-1.41681600	528.7188
C	-2.36458900	-0.61965000	-2.51370500	530.9228
C	-0.30587000	-1.87661200	-2.94638400	552.0486
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C	-0.52066600	-3.39566500	-1.15247300	558.4703
C	-0.08916700	-3.63557800	0.15460900	560.8365
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C	-2.20156600	-2.65791600	1.03953100	562.5049
C	-3.34567700	-0.56211800	0.98925200	563.5601
C	-3.26666300	0.82246700	1.18746700	566.5732
C	-3.18675300	1.74985900	0.05977100	570.1540
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C	-2.20396200	1.72063600	-2.20162300	572.2447
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C	-0.40841400	0.53555400	-3.41944300	576.8480
C	0.31479100	-0.71784900	-3.39532500	577.5012
C	1.73582400	-2.52251900	-1.76293300	588.6979
C	2.39835300	-1.31242300	-2.24009500	591.3076
C	1.69135400	-0.42695500	-3.03645900	592.3876
C	1.82316800	1.00498100	-2.83574800	596.3333
C	0.51529800	1.59603700	-3.06632400	600.5539
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C	-1.32519200	2.74894500	-1.86734500	608.1691
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O	-0.40223300	-1.24285600	-0.00500100	681.6654
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		1078.1174 1086.1794 1097.9114 1126.9420 1127.2725 1128.5799 1129.5868 1132.1089 1152.0687 1186.0842 1199.8263 1209.7984 1224.2240 1227.9283 1236.3453 1237.0701 1251.6949 1257.0384 1260.1746 1267.4180 1274.9334 1278.8202 1283.5625 1285.6692 1302.2624 1306.1578 1307.1719 1320.4508 1322.8099 1327.3598 1328.5939 1334.1480 1335.2037 1338.2160 1340.5955 1369.9283 1376.1343 1376.9049 1379.6818 1383.4491 1385.9956 1391.4276 1395.7470 1414.8431 1432.3514 1442.1452 1448.7659 1454.1800 1460.8579 1462.7511
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C70	C	3.21881800	-2.05291800	-1.25117000	224.7400
	C	2.43895000	-2.96994600	-0.45077100	224.9217
	C	3.96587400	-1.05272600	-0.64171200	251.4000
	C	2.43886200	-2.85823400	0.92355200	251.5511
	C	1.20096500	-3.03066600	1.66166800	260.5787
	C	0.00000000	-3.40533900	1.01354600	305.6181
	C	-1.20096500	-3.03066600	1.66166800	306.3610
	C	3.21863600	0.55570900	-2.33923100	310.3970
	C	2.43894600	-0.48932600	-2.96362900	311.3804
	C	3.96602700	0.28534000	-1.19986400	324.5200
	C	2.43896200	-1.76215100	-2.43282300	333.8299
	C	1.20070200	-2.51671300	-2.36797700	334.4657
	C	0.00000000	-2.01570100	-2.92430400	343.5212
	C	-1.20070200	-2.51671300	-2.36797700	367.7414
	C	0.00000000	-3.52364600	-0.45098300	368.1251
	C	1.20082000	-3.25850400	-1.15117600	391.1095
	C	-1.20082000	-3.25850400	-1.15117600	391.9826
	C	3.21812400	2.39655800	-0.19453000	404.4716
	C	2.43865900	2.66804400	-1.38122100	417.7400
	C	3.96573400	1.22950500	-0.09981900	417.9494
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C	3.21818600	0.92551800	2.21854400	470.5004
C	2.43885300	2.13812400	2.11060800	492.3722
C	3.96591100	0.47501700	1.13802800	493.2474
C	2.43884300	2.85620400	0.93304600	501.1737
C	1.20062000	3.42809100	0.43683000	518.0962
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C	3.21852700	-1.82422300	1.56568300	530.2342
C	2.43889100	-1.34668800	2.68541400	530.7918
C	3.96595300	-0.93555600	0.80307300	544.8302
C	2.43867200	-0.00479700	3.00368600	545.3815
C	1.20076700	0.64377200	3.39544400	548.1086
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C	1.20088800	1.95961100	2.84729100	560.8671
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C	-3.21818600	0.92551800	2.21854400	586.1755
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C	-3.96591100	0.47501700	1.13802700	621.4184
C	-3.21812400	2.39655800	-0.19453000	641.7156
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C	-2.43885300	2.13812400	2.11060800	648.7404
C	-3.96573400	1.22950500	-0.09981900	651.8274
C	-3.21863600	0.55570900	-2.33923100	652.3145
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C	-3.21881800	-2.05291800	-1.25117000	686.5677
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C	-2.43886200	-2.85823400	0.92355200	724.2598
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				728.6100

		732.1822 737.9704 738.9524 741.0252 741.6656 741.7728 742.6188 744.8874 745.9119 746.1532 755.0697 756.8003 757.8902 761.3368 761.6199 761.8721 762.0675 762.2077 764.8130 765.5915 766.4681 766.4715 773.8058 774.6075 777.5340 778.2650 782.8467 783.0433 795.9527 796.7165 797.0018 809.1110 809.4564 843.2827 843.7765 904.5420 913.4591 938.4112 938.7769 948.3262 948.5353 949.1108 979.6608 980.1493 1084.6301 1084.9179 1086.5766 1087.3651 1096.8218 1110.3000
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		1110.6496 1129.4705 1130.5745 1182.4130 1184.0522 1191.8297 1205.1737 1206.2638 1219.0564 1219.3982 1229.5170 1231.5510 1232.1632 1242.1271 1261.9961 1271.1077 1275.3965 1275.8979 1276.4134 1299.7863 1301.8013 1305.5106 1306.5750 1306.6239 1307.0228 1339.8873 1340.3420 1340.4359 1341.8420 1355.6195 1356.5000 1364.5865 1365.6825 1365.6910 1366.4964 1367.3652 1377.0484 1379.5868 1384.4486 1386.7592 1387.9029 1398.4627 1399.5124 1404.2027 1417.6408 1418.0533 1430.6719 1431.3133 1459.9427 1461.9232
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CA@C70	C	-3.20333600	0.72604000	-2.27758100	37.3355
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	C	-3.95084500	0.36590100	-1.16878900	120.2733
	C	-2.44483200	2.80553700	-1.18735900	161.3627
	C	-1.21859300	3.46825600	-0.74964000	165.2147
	C	-0.00976000	3.30459500	-1.48559900	237.2815
	C	1.19534800	3.42799800	-0.74420600	240.4097
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	C	-2.43124800	-1.59111700	-2.53633700	254.6235
	C	-3.95703200	-1.01521500	-0.71480200	269.3125
	C	-2.42699700	-0.27700200	-2.96672300	272.8071
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	C	1.19112200	0.34119700	-3.40661100	326.9951
	C	-0.00509600	2.38923100	-2.64706500	327.4173
	C	-1.19757000	1.71068300	-2.99342700	343.5224

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C	-1.20593300	-2.31869600	2.57431700	454.3544
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C	-0.01029600	3.33225700	1.42862600	549.5645
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C	1.19518700	3.44144200	0.68509400	555.1840
C	3.21094900	0.76646900	2.27087300	560.3978
C	2.42842800	1.98607200	2.24733600	561.8783
C	2.42620600	2.80014200	1.13322100	564.4061
C	3.96830200	0.38936800	1.16820100	565.4005
C	3.22281600	-1.94185000	1.42700100	566.9865
C	2.43175700	-1.53718200	2.56665300	575.8175
C	2.42958000	-0.21947800	2.97853600	577.9256
C	3.97636600	-0.99880000	0.73519200	583.1338
C	3.22360200	-1.96697600	-1.39178400	590.4611
C	2.44408000	-2.94724500	-0.66244600	596.1254
C	2.44377500	-2.93492100	0.71473000	597.2325
C	3.97678600	-1.01174300	-0.71631700	601.5347
C	3.21200300	0.72601400	-2.28300300	621.9190
C	2.43102700	-0.27242600	-2.97366800	642.4860
C	2.43301300	-1.58271000	-2.53888200	642.7695
C	3.96890100	0.36865200	-1.17356200	651.6004

C	3.20621100	2.41124700	-0.02057000	653.0320
C	2.42648400	2.77918700	-1.18104800	653.1553
C	2.42923900	1.94557100	-2.28069700	666.5803
C	3.96274400	1.23570000	-0.01022500	677.6289
C	-0.02521400	-0.15383500	0.00011800	678.8817
O	-0.86843600	-1.00169400	0.00195000	686.7392
O	1.28133800	-0.36192400	-0.00207500	687.1054
H	1.74180900	0.49431500	-0.00044800	690.4248
O	-0.32334800	1.12470100	-0.00022300	692.4342
H	-1.29390100	1.16408200	0.00743700	711.7473
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		844.8019 904.1942 911.6498 932.4038 940.0085 947.1674 948.2094 948.9062 973.3315 974.6811 1076.2475 1080.9455 1087.7570 1089.0189 1097.1893 1107.5712 1107.8118 1110.8703 1120.2856 1122.6319 1173.8485 1181.7966 1190.4928 1202.6429 1204.6348 1213.2223 1216.1694 1221.1254 1226.4167 1231.1404 1232.4167 1257.7418 1259.9042 1266.3634 1268.7373 1269.0038 1273.9132 1294.7936 1298.6236 1302.0795 1304.2308 1307.9364 1310.9089 1322.1517 1331.2862 1331.9703 1334.8706 1337.2163 1351.0862 1353.3342
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		1354.7245 1356.8473 1359.2498 1362.8821 1365.7451 1376.5610 1377.8487 1378.9345 1379.9825 1382.5006 1397.2615 1398.7227 1398.9241 1403.4845 1421.1143 1425.3266 1429.4894 1452.7579 1452.8553 1467.4925 1474.6508 1481.7966 1487.6956 1492.2875 1498.4671 1506.4211 1512.1609 1514.6418 1515.9674 1525.3808 1532.0916 1546.2664 1553.2725 1556.7410 1569.8938 1570.3292 1576.4647 1579.5288 1581.9436 1590.8646 1591.3073 1593.2367 1631.7823 1634.5156 1641.3226 1646.6319 1648.0048 1650.8106 1652.1707 1653.2050
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TS@C70	C	-3.20001400	0.67310300	-2.29335300	-1530.5213
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	C	-3.95399800	0.34093300	-1.18072000	109.5966
	C	-2.43628900	2.76802100	-1.24837000	152.6665
	C	-1.21319200	3.44147800	-0.82543600	170.4388
	C	-0.00593300	3.26345400	-1.55532200	184.2413
	C	1.19907500	3.40412800	-0.81879900	238.3690
	C	-3.22446600	-2.01121200	-1.35119500	240.5846
	C	-2.43548700	-1.65234300	-2.50882300	255.2177
	C	-3.96242500	-1.03015700	-0.69489100	257.9420
	C	-2.42372200	-0.34594100	-2.96158200	268.1106
	C	-1.19142900	0.26068000	-3.41606700	272.9787
	C	0.00071500	-0.48984100	-3.48456400	317.1888
	C	1.19629100	0.25920500	-3.41122000	325.2873
	C	-0.00066700	2.32200500	-2.69504300	326.9616
	C	-1.19209400	1.63736400	-3.02846800	328.0280
	C	1.19392800	1.63125400	-3.02097500	342.9725
	C	-3.23058200	-1.92310100	1.47200500	345.8311
	C	-2.46897500	-2.95436600	0.78582600	346.5642
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	C	-2.46027800	-2.99211000	-0.60188100	368.7954
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	C	1.20296100	-3.21184500	-1.30010100	397.1610
	C	-0.00294700	-1.87616400	-2.99577600	412.0447
	C	-1.20547600	-2.42110200	-2.48452500	418.3831
	C	1.20176900	-2.39974500	-2.46856400	425.1012
	C	-3.20682300	0.82183700	2.24374200	428.3056
	C	-2.43025000	-0.15090900	2.97432200	437.5113
	C	-3.95506000	0.41508200	1.14966200	442.6738
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	C	-1.21079900	-2.25162900	2.63302900	448.8143
	C	-0.00621500	-1.67598600	3.11400700	453.5831
	C	1.19720800	-2.23524300	2.62053500	464.8259
	C	-0.00519600	-3.48641200	0.84517500	470.0404
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	C	1.20047300	-3.12097900	1.50328000	498.1836
	C	-3.21111300	2.41868700	-0.07847600	501.3504
	C	-2.43859600	2.84393800	1.06998200	512.3694
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C	1.18878300	1.82473600	2.91761500	530.8652
C	-0.00573400	-0.26084600	3.51428100	536.9944
C	-1.19905400	0.48336700	3.39583000	539.9179
C	1.19040900	0.48043100	3.39341500	541.3371
C	-0.00840400	3.36246500	1.35166700	545.9392
C	-1.21510200	3.49142200	0.60905400	549.1376
C	1.19792100	3.45193100	0.60830500	550.4164
C	3.21144800	0.81704800	2.25372700	554.3849
C	2.43128800	2.03474100	2.20293800	555.2383
C	2.42673800	2.81717900	1.06969800	562.4297
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C	3.22746100	-1.91185200	1.47694300	564.8849
C	2.43703100	-1.47937300	2.60594600	566.0110
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C	3.23197400	-2.00299800	-1.34565900	588.0670
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C	3.98120400	-1.03108000	-0.68883800	599.5305
C	3.21633200	0.67056900	-2.29340400	621.1489
C	2.43546700	-0.34307300	-2.96092600	640.0772
C	2.44209400	-1.64405800	-2.50132600	641.7984
C	3.96886300	0.33829100	-1.17619000	642.3769
C	3.20648100	2.40144100	-0.07253800	651.4853
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C	2.43450900	1.88832300	-2.31944700	652.7093
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C	0.28753300	0.06925100	-0.03676600	678.0358
O	1.39195500	-0.36333100	-0.01507600	686.0803
O	-0.32165100	1.16111700	-0.00767300	688.2959
H	-1.30894200	0.28094200	0.03393900	689.1305
O	-0.93444900	-0.80643100	-0.09960700	691.7282
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CW@C70	C	-3.20089800	1.96424700	-1.42225300	33.0125
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	C	-2.45097100	3.00605600	0.66537500	171.7299
	C	-1.20720700	3.25302800	1.39557400	189.3298
	C	0.00368600	3.56482600	0.71155400	197.7993
	C	1.20782600	3.19498000	1.37973100	224.9143
	C	-3.19297100	-0.76809900	-2.26462500	239.4741
	C	-2.40943400	0.22832000	-2.96141100	255.0428
	C	-3.93969300	-0.38884800	-1.16385200	262.2860
	C	-2.41308700	1.55416900	-2.56071200	262.6836
	C	-1.18861900	2.33211500	-2.57354800	273.9056
	C	0.00907900	1.75436400	-3.06040400	315.8820
	C	1.21199200	2.29552100	-2.55474400	320.2488
	C	0.00618600	3.55032300	-0.77015700	326.6439
	C	-1.20244000	3.22791700	-1.45209500	331.4103
	C	1.21117100	3.16532300	-1.42693400	336.4215
	C	-3.23769600	-2.44625900	0.01694400	343.2445
	C	-2.46141600	-2.84314800	-1.14546600	348.6997
	C	-3.95280900	-1.24504500	0.00587500	352.5086

C	-2.43585700	-2.00514800	-2.25039900	357.2475
C	-1.19206700	-1.76158600	-2.95688200	366.4240
C	0.00269600	-2.42033300	-2.59189500	370.0936
C	1.20482200	-1.75276600	-2.94772500	379.7424
C	0.01259900	0.34707100	-3.48781600	399.1104
C	-1.18103700	-0.39866600	-3.39261200	399.6720
C	1.20894500	-0.40060700	-3.39056300	417.7864
C	-3.20015800	-0.72798200	2.27026300	422.4810
C	-2.44376200	-1.96449200	2.27932900	426.4150
C	-3.94325000	-0.36821700	1.16006400	437.7681
C	-2.46372500	-2.82048800	1.18809100	438.7856
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C	-0.01662400	-3.28171100	1.47373200	453.4922
C	1.19650200	-3.39807600	0.74273300	457.1808
C	-0.01170800	-3.30395700	-1.41442800	462.2361
C	-1.22631700	-3.48152600	-0.68930500	466.9358
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C	-2.42153700	1.59909200	2.52865700	505.9803
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C	-1.20221200	-1.70895000	2.98464400	535.5364
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C	-0.00106600	1.81092700	3.03557900	543.8510
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C	1.20468600	2.34619600	2.52533200	548.5847
C	3.23333400	-0.73363200	2.29302200	549.1296
C	2.44158600	0.26676800	2.97512500	551.7936
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C	3.99481200	-0.38306000	1.17995400	556.6329
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C	2.45126500	-1.98671900	-2.24425900	573.8185
C	2.44496400	-2.79455500	-1.12938500	580.3123
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C	2.44919300	1.52986600	-2.55749500	600.1265
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C	2.45552400	2.94092300	0.66868600	642.8098
C	2.45419400	2.92129900	-0.70835000	643.0687
C	3.99497000	0.99680700	0.72109500	651.8756

C	-0.80536600	0.04669800	-0.02437300	653.5375
O	-0.93995700	-1.09565900	-0.00395500	656.4815
O	-0.71510400	1.19365600	-0.00452000	678.3793
H	1.55390900	0.73563900	0.30258000	678.9659
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C84	C	-2.56428400	-1.83801000	-2.78243400	212.9633
	C	-3.21875400	-2.20802500	-1.57969800	213.5682
	C	-2.61228700	-3.25595900	-0.85969100	218.7656
	C	-1.28536400	-2.33358900	-3.12835600	224.0351
	C	-0.60853200	-3.27845000	-2.33147000	224.2952
	C	-1.35162800	-3.79372900	-1.23675700	273.5653
	C	-3.98483600	-1.18695000	-0.84957600	277.5176
	C	-4.07031800	-1.27403300	0.56030700	279.5298
	C	-2.63644100	-0.47831100	-3.27629200	284.1436
	C	-3.35227800	0.46770100	-2.60887800	285.6901
	C	-4.06188200	0.12219700	-1.38537700	290.6747
	C	-1.37685100	-0.12400800	-3.88077900	291.6473
	C	-0.84467300	1.18661800	-3.74574200	331.9411
	C	0.55335600	1.27780000	-3.82363800	335.7093
	C	0.84465900	-1.18658800	-3.74575300	344.5489
	C	-0.55337000	-1.27776900	-3.82364600	348.8357
	C	1.37683600	0.12404000	-3.88078100	353.3236
	C	1.58696700	-2.19757500	-2.98435600	356.2081
	C	1.46080800	-3.79713900	-1.12338100	362.1995
	C	0.85685000	-3.23732900	-2.26556000	364.9720
	C	2.85847900	-1.82823900	-2.50595800	367.9332
	C	-3.38327200	2.33920300	-1.28039400	370.4046
	C	-4.07032200	1.27403100	-0.56029500	373.6726
	C	-3.98483300	1.18694900	0.84959300	379.5277
	C	-4.06187400	-0.12219200	1.38539400	380.1063
	C	-2.69060600	3.30098900	-0.59496400	382.5182
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	C	-2.85848800	1.82826000	-2.50593300	438.2759
	C	-1.46081000	3.79714400	-1.12334500	441.5291
	C	-0.85685800	3.23734600	-2.26553300	443.8345
	C	-2.61228000	3.25596200	0.85970300	453.3263
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	C	-2.56427400	1.83800600	2.78244000	458.5950
	C	-2.63642800	0.47831500	3.27630100	462.7587
	C	-3.35227000	-0.46770000	2.60888900	466.4009
	C	0.67895800	4.20718600	-0.02435400	475.7232
	C	-0.67895500	4.20717900	0.02438500	485.7504
	C	-1.35162500	3.79372900	1.23676200	488.0700
	C	-0.60852300	3.27844700	2.33147500	488.4446
	C	-1.28534700	2.33359000	3.12836200	492.0591
	C	1.28535200	2.33361500	-3.12834300	498.7579
	C	0.60852400	3.27846800	-2.33144800	501.1530
	C	1.35162300	3.79373900	-1.23673100	508.8203
	C	-2.69060600	-3.30098900	0.59497200	508.8546
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C	0.55337000	-1.27779800	3.82363300	514.6265
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C	1.58697700	2.19757600	2.98435000	538.1622
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C	2.56428500	-1.83803400	2.78242000	633.4075
C	3.21875500	-2.20803900	1.57968100	637.7190
C	2.61228600	-3.25596600	0.85966600	638.3742
C	2.69060600	3.30098600	0.59499000	644.6899
C	3.38327000	2.33918900	1.28041400	655.9376
C	2.85848900	1.82823700	2.50594600	657.9878
C	2.56427500	1.83803200	-2.78242900	659.1358
C	3.21874800	2.20803800	-1.57969200	664.5401
C	2.61228400	3.25596700	-0.85967600	666.2946
C	4.06187600	-0.12218400	-1.38539200	668.2434
C	3.35226900	-0.46768000	-2.60889300	672.2487
C	2.63642800	0.47833800	-3.27629600	673.6091
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		749.3242 749.4263 751.9604 753.2697 754.9571 761.7854 762.4155 762.6976 763.5611 766.2783 766.7489 767.9211 768.4190 769.5732 772.1604 772.5151 772.8822 773.4725 773.9112 774.5504 776.2216 776.2631 788.1066 790.0001 808.4786 826.3956 835.6551 839.6662 846.8635 860.7585 872.4976 878.0649 879.0844 887.9450 895.5968 916.9171 917.8758 924.0819 947.7718 1034.7989 1036.0441 1036.3506 1043.7213 1044.5770 1046.1694 1054.4923 1064.2739 1067.9219 1144.7157 1147.8946
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		1148.5078 1155.1934 1156.7739 1175.2034 1181.6206 1184.9780 1198.2345 1198.8630 1200.7278 1208.2772 1218.0898 1239.8275 1245.8737 1250.1910 1250.5205 1260.3841 1267.6211 1278.1341 1279.8436 1282.7980 1283.6404 1290.0325 1291.3338 1292.4526 1297.7712 1303.9405 1305.4985 1317.8727 1320.8301 1324.8619 1340.7587 1349.0869 1352.5637 1353.7592 1360.7478 1363.8757 1370.6669 1373.5438 1374.2555 1375.2790 1378.3686 1385.4455 1385.6683 1389.9409 1394.9506 1395.0675 1398.7216 1400.5480 1402.9926 1403.2950
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		1405.1923 1406.3329 1414.8900 1422.1391 1426.7352 1434.3869 1434.6676 1437.9376 1440.4061 1447.6326 1455.6214 1465.1375 1479.1138 1481.5096 1490.2069 1491.8307 1493.3498 1493.4822 1506.8216 1524.3569 1539.2129 1541.0288 1544.7553 1549.7223 1562.2180 1563.1565 1567.3694 1586.2714 1592.7747 1597.0020 1597.8727 1601.2508 1607.1168 1612.0625 1613.7852 1622.6457 1625.5787 1631.8747 1639.4700 1668.1074 1676.3287 1676.7498 1677.6891 1703.4426 1705.0902 1710.2603 1714.4218 1723.8801 1726.7391
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CA@C84	C	-2.51255500	-1.81397900	-2.83169000	44.8330
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	C	0.91652600	-1.17008300	-3.71758500	289.3844
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	C	1.63669100	-2.18697300	-2.94920700	297.5525
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	C	-0.64071400	3.27171200	2.34092000	459.1242
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	C	0.66777100	3.28499900	-2.29145200	477.2553
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	C	0.47173000	-1.30066500	3.82637200	501.0042
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C	1.30797200	-3.80531200	1.24739400	535.6363
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C	-0.69822500	-4.21478500	-0.05234100	539.8603
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C	2.56794900	-0.50791400	3.32606800	564.1122
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C	2.69557000	3.28563700	0.67177300	595.4499
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C	2.64765700	3.24803300	-0.78447000	627.2018
C	4.10052000	-0.13344800	-1.30192000	630.2705
C	3.40637500	-0.46897000	-2.53703700	634.5363
C	2.70991600	0.48378900	-3.21569900	638.0358
C	4.07353900	1.25351800	0.65198500	639.4788
C	4.02323900	1.17493000	-0.76154500	644.6228
C	2.68402400	-3.30425700	-0.55167900	655.4806
C	4.03675600	0.09669700	1.47047400	656.5586
C	3.96266700	-1.20844800	0.92690500	658.5965
C	4.07906000	-1.28801800	-0.48077200	662.4222
C	3.39800000	-2.34487300	-1.21717200	667.4246
C	-0.05296400	-0.13138200	-0.10056100	667.6272
O	-0.50120100	-1.24130100	0.00622900	670.2416
O	1.22715600	0.12753700	-0.36211100	674.0913
H	1.36578900	1.08849300	-0.41491200	682.7146
O	-0.76386600	1.00136700	0.02846500	687.7673
H	-1.68284500	0.74853100	0.22324800	691.6331
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				716.0188
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				719.7643
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		725.3962 726.5330 729.3048 733.6904 739.5235 741.3001 743.5228 746.7307 748.5229 749.2599 749.7316 751.5488 756.0714 757.7054 759.9968 760.9418 763.0111 763.6579 764.2145 764.6151 765.4446 766.3996 768.2095 768.6828 770.4009 772.3873 773.4619 773.8438 776.0683 782.5636 787.5169 789.4904 808.8149 825.9344 835.5446 839.9013 849.1956 863.6484 873.7212 880.2475 881.3595 891.1874 895.7971 918.2541 918.8669 924.0648 947.5447 1034.7922 1038.2697 1038.7805
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		1039.5670 1045.8854 1048.0316 1048.8313 1058.0215 1067.6808 1069.5710 1148.1517 1152.5768 1153.2682 1157.4134 1159.3072 1178.7992 1184.4814 1188.2101 1197.0595 1201.4292 1203.1103 1204.4292 1213.8091 1223.2620 1245.3968 1248.8552 1252.4812 1253.9953 1262.5974 1269.0494 1269.8115 1281.9804 1283.5693 1286.2010 1287.6096 1292.2500 1297.6144 1298.6465 1301.3934 1305.1576 1310.0484 1323.6921 1324.6723 1330.3288 1342.4121 1353.1131 1356.4498 1357.2171 1365.4939 1366.4236 1373.3287 1376.7784 1377.1572
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TS@C84	C	2.56852300	1.91329400	-2.72728600	-1645.7047
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	C	1.25827100	3.83074200	-1.21187300	114.4232
	C	3.98948700	1.31285800	-0.77802900	133.7465
	C	4.04047500	1.40598000	0.63504100	213.7880
	C	2.69871100	0.55724600	-3.21516000	217.8674
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	C	4.05697600	0.25411900	1.46440800	357.9223
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	C	1.73444800	-2.14237200	-2.93921200	365.9000
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C	-1.19682900	-3.83789200	-1.25191200	468.5286
C	2.57695300	3.38211700	0.63983700	477.6528
C	3.29470900	2.44693600	1.33803600	486.1593
C	2.76048500	1.91970800	2.55163800	489.8733
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C	1.32078600	3.83990900	1.14281700	509.9292
C	-1.35424800	-3.84622200	1.10283300	510.8402
C	-0.78778300	-3.26308500	2.25240700	512.0639
C	-1.56546300	-2.24805300	2.95421500	512.1891
C	-0.86800100	-1.20915500	3.72039900	515.1920
C	0.53117100	-1.25286300	3.82742000	520.0756
C	-1.44314400	0.08377700	3.84195300	523.1667
C	-1.41174200	2.29796100	3.09445300	527.8406
C	-0.75543800	3.26886100	2.31289600	529.4341
C	-1.49797500	3.76907500	1.20812400	530.3099
C	-0.81251900	4.19604300	0.00592300	534.9538
C	0.54702200	4.22726300	-0.01707000	538.9721
C	-3.37279000	-0.57785800	2.53915600	541.1083
C	-2.70142400	0.39554000	3.21472400	553.5815
C	-2.66644300	1.75878600	2.72485100	556.2177
C	-3.31373200	2.11335300	1.51422200	579.1862
C	-2.73523200	3.19024900	0.80781300	586.6696
C	-2.59615500	-3.40265800	0.55139500	591.4923
C	-3.33333200	-2.46120400	1.22206700	596.0967
C	-2.84082800	-1.92538500	2.45224500	607.9647
C	-2.43983500	-1.92597600	-2.82012700	616.7308
C	-3.11379100	-2.32443800	-1.63627100	617.2472
C	-2.48927000	-3.35453000	-0.90351800	629.9170
C	-4.02176200	-0.01394800	-1.45657600	633.2420
C	-3.29924000	0.35590600	-2.66327900	637.1979
C	-2.54160500	-0.56847300	-3.31394200	638.5966
C	-4.03663100	-1.41414200	0.48591100	638.7716
C	-3.92476500	-1.32480400	-0.92266800	644.7086
C	-2.78480200	3.22954300	-0.65054900	655.1519
C	-4.07098600	-0.25651400	1.30535100	656.8541
C	-4.02371600	1.05868600	0.77365400	658.8355
C	-4.08287200	1.14158000	-0.63641600	663.9668
C	-3.42310600	2.23314100	-1.34332600	666.8864
C	-0.92569600	0.11152900	0.03836700	667.7137

O	-1.11517400	-1.03513300	0.08995600	670.9285
O	-0.79281800	1.26592300	0.01389100	673.5853
H	1.79649600	0.41876100	0.26352200	682.4378
O	1.42111100	-0.27269900	-0.29996000	687.5858
H	1.45278700	-1.07898100	0.23576600	692.0078
				693.9614
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				701.5664
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				717.9390
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				742.2082
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				747.3421
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				776.1829
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				790.2202
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				826.4799
				830.5995

		835.7424 839.8511 847.5475 861.5021 872.6791 879.5180 879.6423 889.2962 895.3886 917.4750 918.3419 923.8589 947.5974 1024.7586 1036.2581 1036.6348 1037.8253 1044.7715 1045.6096 1047.8257 1056.6858 1065.2873 1068.5070 1145.7756 1149.7974 1150.0286 1155.6220 1157.2327 1177.0280 1181.9657 1187.1587 1199.4836 1200.9009 1202.3599 1209.7809 1219.4714 1241.2464 1246.0207 1251.1447 1251.7918 1260.8541 1267.5612 1272.9500 1279.9788 1280.8206 1283.7379 1285.6793 1290.9485 1293.3070 1294.8931
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		1299.5293 1305.1778 1307.2199 1319.1050 1322.9297 1326.1194 1336.2565 1342.1306 1350.7871 1353.6516 1355.1042 1362.8258 1365.4750 1371.9622 1374.9453 1375.2484 1376.2402 1379.8379 1387.1651 1388.1876 1392.2440 1395.4229 1396.6013 1400.2250 1402.6470 1404.6410 1405.6900 1407.4680 1409.3076 1416.5300 1423.7402 1428.4638 1435.9168 1437.1825 1439.0922 1443.2036 1449.1169 1457.8555 1467.6058 1481.1950 1483.9286 1492.0433 1493.2210 1495.6404 1496.2250 1508.5828 1525.7077 1539.8512 1542.8473 1547.3602
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					1551.8152 1563.3142 1564.7977 1568.7542 1585.8321 1593.9602 1597.8619 1599.7246 1601.0223 1608.0274 1613.3164 1616.0371 1623.8262 1627.0843 1633.5196 1641.2133 1667.1992 1674.9273 1677.5523 1679.6683 1703.4539 1706.5895 1711.7882 1715.9821 1721.8582 1726.2878 2018.3019 2217.0311 3720.9777
CW@C84	C	2.56852300	1.91329400	-2.72728600	33.0867
	C	3.19021600	2.30552000	-1.51693600	57.1165
	C	2.52971100	3.33308700	-0.81294900	63.5597
	C	1.27916700	2.36673700	-3.09431000	98.3430
	C	0.55308200	3.29254500	-2.31779800	121.8852
	C	1.25827100	3.83074200	-1.21187300	156.7643
	C	3.98948700	1.31285800	-0.77802900	184.9814
	C	4.04047500	1.40598000	0.63504100	214.7744
	C	2.69871100	0.55724600	-3.21516000	216.5187
	C	3.44455200	-0.36283100	-2.54347700	223.6944
	C	4.13162800	0.00558000	-1.31213300	225.7663
	C	1.46113700	0.16347800	-3.83898300	230.3926
	C	0.97052300	-1.16020900	-3.71091500	256.7251
	C	-0.42288300	-1.29678600	-3.81552400	276.3660
	C	-0.79713300	1.15497800	-3.74833300	281.7834
	C	0.59784600	1.28830500	-3.79977600	283.5584
	C	-1.28190500	-0.17236400	-3.89167400	287.0036
	C	-1.58798700	2.14488700	-3.00825800	291.7500
	C	-1.56061500	3.76397500	-1.15737600	297.7196
	C	-0.91174700	3.21414700	-2.28226100	302.3338

C	-2.85477000	1.73361900	-2.55341500	310.3600
C	3.51521200	-2.23103900	-1.21303600	331.5289
C	4.16750200	-1.14695300	-0.48365900	336.6548
C	4.04487000	-1.05984400	0.92809300	345.0954
C	4.05697600	0.25411900	1.46440800	349.4883
C	2.82956400	-3.20885500	-0.53873700	359.9161
C	1.73444800	-2.14237200	-2.93921200	361.5573
C	2.99095400	-1.73639300	-2.44557200	362.8636
C	1.62035300	-3.73936400	-1.08457700	369.0726
C	1.01851700	-3.19956100	-2.23460800	371.5514
C	2.71853600	-3.16422500	0.91369800	376.2468
C	3.28515300	-2.09986300	1.64510000	382.5986
C	2.58417800	-1.74851100	2.83113200	383.8365
C	2.59958300	-0.38813500	3.32400100	388.6762
C	3.30082200	0.57792300	2.66862200	391.5435
C	-0.53188200	-4.22108700	-0.02778700	405.9939
C	0.82565800	-4.17300600	0.04438400	430.7959
C	1.46193300	-3.73788500	1.26576800	442.3295
C	0.67775600	-3.24898500	2.34292000	444.5707
C	1.31154300	-2.28274000	3.14980900	448.4497
C	-1.13618200	-2.37440900	-3.13719100	457.4724
C	-0.44420400	-3.29336500	-2.32636600	460.2405
C	-1.19682900	-3.83789200	-1.25191200	462.1499
C	2.57695300	3.38211700	0.63983700	462.3906
C	3.29470900	2.44693600	1.33803600	468.5824
C	2.76048500	1.91970800	2.55163800	472.1192
C	1.31583900	-0.07379800	3.89991500	478.9361
C	-0.65777200	1.26462000	3.79875000	486.4789
C	0.74396600	1.21783700	3.75076200	492.3256
C	1.46555300	2.24908700	3.00300700	493.0003
C	0.71249100	3.26516800	2.27301600	495.6454
C	1.32078600	3.83990900	1.14281700	500.2714
C	-1.35424800	-3.84622200	1.10283300	502.9828
C	-0.78778300	-3.26308500	2.25240700	508.5675
C	-1.56546300	-2.24805300	2.95421500	510.8823
C	-0.86800100	-1.20915500	3.72039900	511.4914
C	0.53117100	-1.25286300	3.82742000	513.8447
C	-1.44314400	0.08377700	3.84195300	514.9720
C	-1.41174200	2.29796100	3.09445300	516.1581
C	-0.75543800	3.26886100	2.31289600	523.1839
C	-1.49797500	3.76907500	1.20812400	526.3439
C	-0.81251900	4.19604300	0.00592300	529.5832
C	0.54702200	4.22726300	-0.01707000	530.5368
C	-3.37279000	-0.57785800	2.53915600	531.7041
C	-2.70142400	0.39554000	3.21472400	538.1357
C	-2.66644300	1.75878600	2.72485100	543.0095
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C	-2.73523200	3.19024900	0.80781300	556.4666
C	-2.59615500	-3.40265800	0.55139500	582.3359
C	-3.33333200	-2.46120400	1.22206700	587.9691

C	-2.84082800	-1.92538500	2.45224500	593.3404
C	-2.43983500	-1.92597600	-2.82012700	595.2965
C	-3.11379100	-2.32443800	-1.63627100	608.2429
C	-2.48927000	-3.35453000	-0.90351800	608.7199
C	-4.02176200	-0.01394800	-1.45657600	617.6630
C	-3.29924000	0.35590600	-2.66327900	617.9974
C	-2.54160500	-0.56847300	-3.31394200	629.8951
C	-4.03663100	-1.41414200	0.48591100	634.6753
C	-3.92476500	-1.32480400	-0.92266800	638.1365
C	-2.78480200	3.22954300	-0.65054900	639.5530
C	-4.07098600	-0.25651400	1.30535100	645.2537
C	-4.02371600	1.05868600	0.77365400	647.3367
C	-4.08287200	1.14158000	-0.63641600	655.7901
C	-3.42310600	2.23314100	-1.34332600	657.3061
C	-0.92569600	0.11152900	0.03836700	660.1289
O	-1.11517400	-1.03513300	0.08995600	664.3744
O	-0.79281800	1.26592300	0.01389100	667.4302
H	1.79649600	0.41876100	0.26352200	668.9983
O	1.42111100	-0.27269900	-0.29996000	672.3348
H	1.45278700	-1.07898100	0.23576600	674.8845
				682.9746
				687.7898
				692.6601
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				702.1782
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				749.4809
				750.6003
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				758.9431
				759.8724
				762.2125
				762.9879
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		765.3244 765.6895 767.0176 767.9684 768.7307 769.7480 771.0718 772.4798 773.5281 773.6702 774.6970 775.1222 787.1508 789.1250 809.0641 825.4840 835.1875 840.0469 846.4467 861.6700 873.2940 879.3494 880.5497 889.5954 895.2717 917.7271 918.3566 922.6368 947.6288 1034.9903 1036.3038 1037.6665 1043.6615 1045.6485 1048.2048 1057.0622 1065.6928 1068.5186 1144.6693 1150.8604 1151.8983 1154.0628 1155.7260 1176.2310 1180.8862 1187.3221 1199.9825 1201.5655 1202.6351 1211.3183
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		1218.5453 1242.4413 1244.3980 1250.7438 1251.5355 1260.8193 1267.0646 1279.1932 1280.4932 1283.7021 1285.4887 1290.5572 1295.4277 1295.8351 1299.7659 1303.3306 1307.5067 1320.1608 1323.2924 1326.6497 1339.2826 1351.9794 1353.2686 1354.7831 1362.3780 1364.1621 1370.5700 1372.2406 1374.0869 1375.0818 1378.4045 1387.0364 1388.9630 1391.5387 1392.0042 1395.8701 1399.3766 1401.0178 1405.0747 1406.5573 1407.9061 1409.4454 1414.5130 1420.5792 1423.2782 1427.4439 1435.5566 1436.7126 1437.2826 1443.0531
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					1447.6098 1457.6916 1468.2261 1480.7142 1483.3569 1491.5287 1492.2954 1496.2656 1497.2436 1508.5721 1524.5093 1539.0604 1542.3084 1545.7758 1552.0246 1560.4013 1565.5533 1566.9152 1581.0168 1591.9966 1596.2013 1597.8702 1598.9336 1607.7866 1609.3946 1611.0316 1615.5966 1621.6041 1626.1202 1631.2674 1639.4421 1659.5804 1668.0757 1668.9237 1671.1202 1699.4240 1701.0068 1705.7430 1709.2166 1714.0815 1716.9103 2465.1751 3802.3955 3909.5472
CA_WM @C70	C	3.24373700	2.29903700	0.71591200	42.0373
	C	2.44500700	2.99872400	-0.28482700	71.5680
	C	4.00238300	1.17788700	0.38057500	104.1476
	C	2.42622300	2.56426500	-1.59318900	143.9985
	C	1.19321400	2.59686900	-2.37784100	233.4779

C	-0.00811100	3.16304000	-1.85413600	241.3399
C	-1.21656900	2.59467600	-2.36226700	248.6700
C	3.28059300	0.02347800	2.43913300	255.2139
C	2.48333900	1.19842100	2.77335400	259.7253
C	4.03000800	0.00657000	1.25884800	269.2312
C	2.46421400	2.30070700	1.93439800	276.9013
C	1.21560200	3.01248800	1.67154700	284.7412
C	0.01349700	2.65193800	2.32322800	296.7503
C	-1.19194300	3.00897300	1.67357300	333.4211
C	0.00086500	3.61784200	-0.43225300	339.3259
C	1.20856700	3.47534300	0.31926200	340.6493
C	-1.20014400	3.47496700	0.32422900	342.2833
C	3.22604400	-2.29401400	0.76380900	344.3081
C	2.44832000	-2.26197700	1.97937600	357.0234
C	3.98799200	-1.18044700	0.40565000	360.0769
C	2.46998400	-1.13545300	2.78785400	362.7290
C	1.21970400	-0.67437800	3.37049400	370.7301
C	0.00890000	-1.40130600	3.23491800	373.5654
C	-1.20240700	-0.67381000	3.37868700	397.2547
C	0.01584700	1.47431500	3.19881500	400.5004
C	1.22482700	0.75051400	3.35605300	424.6361
C	-1.19703300	0.75041700	3.35836900	432.5310
C	3.18416300	-1.44506200	-1.91385300	438.8579
C	2.42557300	-2.62479000	-1.54573400	444.6818
C	3.94717900	-0.74458700	-0.97846300	450.8557
C	2.44282900	-3.03181800	-0.22219500	452.9607
C	1.19858900	-3.48951400	0.39903000	455.4918
C	-0.01721400	-3.62660300	-0.35058900	460.0284
C	-1.21953300	-3.45609200	0.40608200	466.3198
C	-0.00032300	-2.59984600	2.38817400	474.5479
C	1.20172400	-2.98138200	1.74393800	475.4857
C	-1.21144700	-2.96770000	1.74787500	498.5863
C	3.18549400	1.37924700	-1.93897100	503.6279
C	2.39503900	0.64861600	-2.89823200	504.9864
C	3.95448100	0.70448700	-0.99437900	515.8645
C	2.39621800	-0.73520900	-2.88990100	523.0329
C	1.17591800	-1.48282400	-3.14372100	526.1678
C	-0.02038200	-0.78485900	-3.44361100	528.2169
C	-1.21911400	-1.46182300	-3.10950700	530.2051
C	-0.01998700	-3.20200600	-1.78093100	533.5586
C	1.18877400	-2.66885800	-2.32999000	537.2116
C	-1.22627800	-2.63566600	-2.29284500	545.9672
C	-0.01959500	0.70038400	-3.45834400	547.9874
C	1.17786500	1.39642400	-3.16534200	552.9778
C	-1.21449500	1.39631300	-3.14885200	556.4674
C	-3.23608700	-1.42531400	-1.88526600	557.3614
C	-2.44457800	-0.71801400	-2.86212100	559.0058
C	-2.44097600	0.66218800	-2.87775300	561.5118
C	-4.00680400	-0.72995000	-0.95014300	563.4117
C	-3.26393800	-2.28474600	0.79539000	566.2610

C	-2.47159500	-3.00631300	-0.19458500	568.2155
C	-2.46072600	-2.59283300	-1.51065100	571.2894
C	-4.03642300	-1.17130700	0.43888600	575.6919
C	-3.27193000	0.03231400	2.45441200	583.3202
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C	-2.46206900	-2.25464800	1.99920500	595.8903
C	-4.04748600	0.02051800	1.28743800	599.2934
C	-3.23895500	2.30118100	0.73351100	604.0463
C	-2.43775200	2.29519400	1.93558900	609.1829
C	-2.45718700	1.19652100	2.77600200	621.0225
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C	-3.22909700	1.39490500	-1.91706000	641.7778
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C	-4.00201100	0.72280100	-0.96832100	652.7243
C	0.73847700	0.10164200	-0.16301800	656.8793
O	1.67821600	0.10838100	0.56845900	660.8922
O	0.09704700	1.14390900	-0.55362500	675.2061
H	-0.86672200	0.87528300	-0.53640900	677.2319
O	0.22608600	-1.03097400	-0.60142000	685.8829
H	0.73218900	-1.71649000	-0.14308900	688.5081
H	-1.53343900	-0.86116200	-0.06757700	691.5804
H	-1.23842800	0.01861400	1.14685800	694.1688
O	-1.74308600	-0.00288900	0.32155500	700.8685
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				738.6125
				740.9729
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				744.7770
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				747.3768
				749.2980
				750.7699
				752.2034
				753.4988
				755.4498
				756.2261
				759.0147
				761.8173
				763.7441
				765.8142
				768.5533
				769.7219
				772.2581

		772.9000 775.6992 776.8835 778.1828 780.1324 782.5601 783.7105 784.2205 788.8087 793.7284 794.3417 795.7014 797.7281 806.4802 808.9160 839.5631 843.1004 895.1571 902.1025 921.9851 927.3680 932.0531 933.5038 945.9101 960.7345 965.1012 975.4260 1057.8285 1061.5755 1066.5743 1068.0669 1080.6886 1096.1697 1096.9035 1099.4000 1108.3603 1144.2625 1160.7449 1175.6387 1177.1573 1187.2908 1190.1881 1194.4682 1196.5242 1200.8984 1207.3526 1210.5364 1223.1054 1243.6826 1248.3709
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		1251.1008 1252.4745 1256.9096 1266.5028 1279.3715 1281.9297 1283.3130 1290.4081 1293.6567 1304.3705 1311.5191 1315.3201 1321.6723 1323.5052 1327.3277 1331.7176 1334.1850 1334.3857 1337.1121 1346.2752 1347.9826 1350.4221 1355.8737 1362.0956 1364.3503 1372.4370 1374.7733 1380.4992 1383.7847 1391.2185 1396.8824 1401.2462 1406.0605 1424.5119 1427.2060 1429.7970 1439.8264 1446.7386 1454.0327 1459.6511 1466.6140 1470.5034 1482.2918 1490.0672 1491.8072 1497.5978 1502.3479 1517.4593 1532.1229 1540.7789
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					1548.6005 1553.0544 1554.3076 1564.3081 1568.6530 1570.0610 1575.4808 1576.3219 1602.8280 1609.3273 1624.5638 1627.7816 1629.4098 1632.7505 1635.6320 1639.6324 1640.5074 1642.3209 1647.4617 1651.1211 1656.2094 2026.5595 3160.7667 3756.2556 3820.0660 3892.3462
CA_WM @C84	C	2.35981200	2.15843900	-2.71158700	31.7238
	C	2.96669400	2.56931000	-1.49988100	67.4545
	C	2.25106500	3.53966800	-0.76650000	91.1261
	C	1.03704000	2.52935800	-3.06232000	120.1139
	C	0.26249000	3.39824300	-2.26101500	152.7194
	C	0.94486800	3.96770200	-1.14388900	160.2688
	C	3.83866000	1.61482400	-0.79446600	170.4342
	C	3.90898300	1.67761700	0.61242000	207.0401
	C	2.58182500	0.82609800	-3.23028300	220.3211
	C	3.39891100	-0.05216900	-2.58449000	223.8487
	C	4.07116900	0.33436300	-1.35641700	224.8843
	C	1.37118600	0.35837600	-3.85208900	230.7027
	C	0.98693400	-1.00189000	-3.75347900	258.8785
	C	-0.39327100	-1.23985400	-3.85899100	265.0182
	C	-0.95596700	1.17283500	-3.73486700	284.0557
	C	0.42550100	1.41457700	-3.78426900	289.0383
	C	-1.34221100	-0.18519800	-3.91345100	290.8555
	C	-1.80279700	2.08265600	-2.95335700	293.8336
	C	-1.84949000	3.64333900	-1.04355100	299.2595
	C	-1.19281400	3.18627200	-2.20454800	304.7243
	C	-3.02417600	1.55822300	-2.48718100	306.2893
	C	3.66527700	-1.95274200	-1.31696000	331.5407
	C	4.22877800	-0.83215600	-0.56575400	336.1870

C	4.12867700	-0.78826100	0.84773400	342.7471
C	4.03630400	0.51159500	1.40873100	344.8476
C	3.08440200	-3.00741300	-0.65983300	350.0507
C	1.84240400	-1.94376800	-3.01724900	362.6718
C	3.07040300	-1.46153300	-2.52319600	364.2037
C	1.90125500	-3.60224800	-1.20521100	367.6787
C	1.23092000	-3.07581500	-2.33191300	375.9446
C	2.99413800	-3.00241900	0.80127900	377.7535
C	3.47852900	-1.90862100	1.55237700	381.0390
C	2.76316900	-1.62880600	2.75081300	384.8509
C	2.67496400	-0.28077600	3.27345500	391.3062
C	3.28033900	0.75152800	2.62851100	393.1239
C	-0.19483500	-4.24550500	-0.12741900	394.4069
C	1.15781700	-4.10995400	-0.07147900	430.0005
C	1.78315400	-3.66437900	1.15424900	446.6045
C	0.97468600	-3.25404700	2.25236600	449.0889
C	1.53720900	-2.26141400	3.07631600	452.9016
C	-1.00570600	-2.38343000	-3.19123500	459.9565
C	-0.22498900	-3.26333100	-2.40870900	462.8481
C	-0.90792800	-3.88031500	-1.33052700	469.3442
C	2.31725500	3.55301600	0.68880000	472.3035
C	3.10477900	2.64600500	1.34871100	475.4279
C	2.63638300	2.05135000	2.55439700	478.2045
C	1.37810000	-0.07759200	3.87270400	484.7605
C	-0.69443200	1.10680500	3.85890000	486.1797
C	0.70328200	1.16863400	3.76746100	493.6293
C	1.33213900	2.27241500	3.03293400	496.2375
C	0.50099200	3.25355800	2.34456400	496.8926
C	1.04419800	3.91187800	1.22237400	499.9263
C	-1.02252300	-3.95066000	1.02355800	502.7665
C	-0.48958200	-3.36412300	2.18636600	507.7582
C	-1.33927200	-2.43889700	2.94186600	510.5152
C	-0.71713700	-1.37113900	3.73335500	511.8392
C	0.68681500	-1.31024600	3.79288700	514.0299
C	-1.39287900	-0.13034400	3.90588600	514.6740
C	-1.53148200	2.09455100	3.18090100	518.1879
C	-0.95776800	3.12707700	2.40582900	524.9513
C	-1.74439300	3.58739900	1.31750800	527.3044
C	-1.12220800	4.11616600	0.11946400	530.4485
C	0.22792900	4.27802200	0.07919000	532.5042
C	-3.29644100	-0.90337200	2.60719500	534.6591
C	-2.68523300	0.10086300	3.30168300	539.5613
C	-2.75060800	1.47276200	2.82741300	542.9494
C	-3.42461600	1.79348000	1.61991200	544.0249
C	-2.92983500	2.91398100	0.92230800	546.1505
C	-2.29791400	-3.58044100	0.50100000	547.5141
C	-3.09986600	-2.72644400	1.21302900	558.3500
C	-2.64910500	-2.20010000	2.46750500	576.9707
C	-2.33640200	-2.04563700	-2.85309400	582.4467
C	-2.94200300	-2.50991500	-1.65507700	591.0741

C	-2.22277600	-3.49411500	-0.95154000	594.4858
C	-4.02784200	-0.29545300	-1.40962500	595.3545
C	-3.37176000	0.15498000	-2.63280900	597.8266
C	-2.56100600	-0.69193100	-3.32694400	607.7743
C	-3.89277200	-1.72516600	0.51121300	616.7027
C	-3.81266700	-1.59785300	-0.90007400	616.8622
C	-3.00852200	2.98792500	-0.53084800	629.7255
C	-4.01770800	-0.60462800	1.37184200	633.4249
C	-4.06845700	0.71484700	0.85924800	634.8980
C	-4.15369400	0.82345100	-0.55107200	637.6950
C	-3.58820700	1.97316600	-1.24353000	638.7765
C	-0.67458400	0.35951500	-0.09296900	645.0971
O	-1.00555200	-0.20337900	-1.10885700	654.6365
O	0.01653000	1.47669100	0.00239800	659.6744
H	0.41119200	1.63437200	-0.87018800	660.2421
O	-0.94859500	-0.09945500	1.12229400	665.5705
H	-1.48553600	-0.89781400	0.99372200	666.2600
H	1.24233800	-0.89119200	0.83520000	668.8672
H	0.89175300	-1.38097200	-0.57411800	673.4575
O	1.46648100	-0.76648300	-0.09733200	675.0645
				681.5050
				687.9250
				692.9215
				693.8583
				694.0531
				699.3435
				700.9210
				702.6386
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				718.7112
				719.4515
				721.1572
				721.4091
				728.0732
				728.1926
				733.1529
				735.0511
				741.7431
				744.1004
				746.0669
				748.5201
				749.2267
				750.5615
				752.5670
				753.8294
				758.1503
				760.7116
				761.0515
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				763.9410

		765.9223 766.6762 767.1977 769.0092 769.5783 771.0260 771.5548 772.8371 774.0017 775.1027 779.3701 779.5994 787.0321 788.4556 804.9948 808.0304 824.8042 834.0299 838.3050 844.1873 858.6762 872.1608 874.5483 877.8218 885.8729 894.6794 914.0630 915.4713 921.7184 947.2098 1030.2781 1031.7459 1032.9035 1040.3762 1041.9637 1043.2345 1050.1155 1060.5436 1064.5131 1078.8708 1140.1916 1142.2787 1145.3025 1151.8423 1153.0655 1167.4411 1175.8728 1180.2216 1191.4685 1193.9368
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		1198.7999 1200.2205 1205.1819 1215.1127 1235.0418 1240.1613 1245.3009 1246.1360 1254.8602 1264.5382 1271.2508 1275.8049 1277.5208 1279.8194 1285.3570 1287.1530 1289.9387 1292.8138 1297.7367 1302.7487 1311.3575 1314.2672 1315.9845 1322.3550 1335.3665 1345.4340 1347.0478 1350.3323 1355.4658 1357.2909 1363.6352 1366.3738 1369.4058 1370.2043 1372.1070 1378.0685 1381.5490 1382.8175 1388.5484 1389.3257 1391.1908 1394.8891 1398.4340 1399.2239 1399.5062 1400.8474 1410.5352 1415.4784 1421.9939 1427.2153
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		1430.0975 1432.6418 1435.0200 1443.7981 1450.9454 1460.1198 1472.5656 1475.6758 1484.5596 1485.6575 1487.9804 1489.8297 1501.3059 1518.7720 1532.1417 1535.3270 1538.6543 1544.9324 1549.4043 1557.8883 1559.4129 1561.9642 1579.7515 1586.0110 1590.0079 1593.4996 1596.0183 1600.5708 1607.4049 1608.3665 1617.3461 1619.5869 1626.5302 1633.3005 1634.7267 1659.7059 1666.3248 1671.0537 1675.5661 1691.0486 1702.5696 1704.5356 1712.2919 1716.4130 1719.4510 1894.8523 3797.8927 3816.9449 3828.4851 3917.9204
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TS_WM@ C84	C	-2.50929100	1.85060300	2.79122800	-739.1866
	C	-3.06635000	2.37661200	1.60195400	41.2015
	C	-2.32624200	3.41740000	1.00145300	74.7487
	C	-1.20897600	2.19122200	3.22824300	101.1739
	C	-0.40933400	3.13123300	2.54986700	139.6859
	C	-1.04367300	3.80702200	1.47404100	155.0842
	C	-3.90283700	1.49445200	0.76998100	168.3375
	C	-3.90332300	1.70010000	-0.62851500	187.5319
	C	-2.74226000	0.47085100	3.16420300	219.7448
	C	-3.53388600	-0.34300700	2.40941900	221.8169
	C	-4.16049300	0.16306800	1.19480400	230.4408
	C	-1.55515500	-0.05088900	3.79335900	234.8033
	C	-1.15114600	-1.39366100	3.58978100	248.0362
	C	0.22900100	-1.63537100	3.73757300	282.1183
	C	0.76287800	0.78845400	3.84782400	285.1478
	C	-0.61949800	1.01420300	3.86159400	290.3529
	C	1.15837500	-0.57656200	3.91747600	294.8613
	C	1.63044500	1.77598200	3.19543700	295.7808
	C	1.75552300	3.52318400	1.47267500	307.1293
	C	1.04460300	2.94233600	2.53932700	308.5429
	C	2.87885900	1.31904300	2.73789700	331.2004
	C	-3.70755200	-2.10209200	0.94265700	336.1141
	C	-4.26961900	-0.92081300	0.28171600	344.7615
	C	-4.09651300	-0.72976700	-1.11838300	349.7453
	C	-3.98279400	0.62072600	-1.54480300	361.4201
	C	-3.06101700	-3.06593900	0.20854400	362.7546
	C	-1.96072500	-2.25745400	2.71977200	366.6118
	C	-3.17654000	-1.73523300	2.22069300	372.7400
	C	-1.89718200	-3.70415700	0.74238100	375.7418
	C	-1.29431000	-3.30138300	1.95147200	380.8488
	C	-2.90312600	-2.91473000	-1.23660300	383.5927
	C	-3.37901800	-1.76083700	-1.89884700	388.7069
	C	-2.60538000	-1.35722000	-3.02800200	392.9194
	C	-2.51243700	0.03501300	-3.41289100	397.1279
	C	-3.16712200	0.98944100	-2.69746100	427.8263
	C	0.25199400	-4.23156300	-0.29449400	440.0889
	C	-1.09780000	-4.09562600	-0.39775100	446.4420
	C	-1.66803100	-3.53124800	-1.59855000	448.7741
	C	-0.81535900	-3.00911200	-2.60964500	453.7879
	C	-1.35520800	-1.94344700	-3.35394300	460.3776
C	0.89006900	-2.70235800	2.99119500	464.5837	
C	0.15857900	-3.49834600	2.08085300	465.7462	
C	0.90045900	-3.99128500	0.97407100	469.8518	
C	-2.32508900	3.57983300	-0.44431200	477.9319	
C	-3.07474400	2.74305400	-1.22712200	478.8166	
C	-2.54287400	2.27787700	-2.46338000	485.8781	
C	-1.19113900	0.30624600	-3.92518000	490.6993	
C	0.86819200	1.49425800	-3.67723400	493.6098	
C	-0.53584200	1.53799400	-3.65932200	496.6788	
C	-1.21627900	2.55410800	-2.85437500	499.6448	

C	-0.42599400	3.46200100	-2.03288000	501.9507
C	-1.03105400	3.99777000	-0.88028300	503.0781
C	1.13022600	-3.81808200	-1.36919300	507.5519
C	0.64400100	-3.11468100	-2.48473800	508.8500
C	1.51317800	-2.10779800	-3.08990500	512.2413
C	0.91156100	-0.97391100	-3.79366900	513.7393
C	-0.48619600	-0.92110500	-3.93119000	514.1245
C	1.58288500	0.27683700	-3.80749700	517.9022
C	1.67005400	2.42084600	-2.88380300	524.9659
C	1.03917500	3.35809500	-2.03913800	526.1147
C	1.77051100	3.71391700	-0.87844900	530.7019
C	1.07836000	4.10441300	0.33320400	532.4395
C	-0.27331800	4.24701000	0.32837300	534.9267
C	3.44666400	-0.60419500	-2.53203000	538.6167
C	2.85595400	0.46015900	-3.14693900	541.2249
C	2.89018500	1.78508900	-2.54842200	545.4094
C	3.51430200	1.99232600	-1.28888300	546.7272
C	2.95578100	3.02424600	-0.50307900	558.8435
C	2.37593300	-3.49241900	-0.75740400	578.3130
C	3.19506000	-2.55669800	-1.33608600	584.8740
C	2.79428300	-1.90560800	-2.54136000	589.7435
C	2.23134500	-2.31138000	2.73573400	593.9442
C	2.90316000	-2.64028000	1.52262800	597.6380
C	2.22783100	-3.55552200	0.69162800	607.4120
C	3.96637400	-0.39913700	1.53806300	616.0646
C	3.23013400	-0.08626800	2.75547700	616.4856
C	2.40781900	-1.00597600	3.33805500	618.9981
C	3.95604900	-1.63011900	-0.51158300	629.7094
C	3.79698700	-1.64679200	0.89770700	633.5616
C	2.95448900	2.94522700	0.95225400	637.0815
C	4.12199400	-0.42788200	-1.24908500	638.4362
C	4.14010600	0.84066800	-0.61139100	644.6552
C	4.13463500	0.80323800	0.80524000	654.5811
C	3.51307100	1.86781200	1.58213600	657.8482
C	0.70672500	0.48855700	0.01453600	660.8581
O	1.47085900	0.13356900	-0.84650400	664.3855
O	-0.09858000	1.41487800	0.18182700	666.5926
H	-1.36435300	0.44441200	0.03438000	670.1607
O	0.52594900	-0.56360800	1.07144400	671.3107
H	1.15553900	-1.27318000	0.84868800	673.9965
H	-1.58352600	-0.92095200	-0.80100900	675.4802
H	-0.63650200	-0.81921000	0.68927200	682.1530
O	-1.59693600	-0.54565100	0.09779000	686.9725
				691.2482
				692.9630
				694.6349
				698.2832
				700.4266
				702.2167
				713.4061

		718.5278 719.9549 720.2195 720.6514 727.5998 727.8164 732.2139 736.0551 741.7482 743.3974 745.0013 749.1204 749.3106 751.2267 751.2895 753.0504 758.5614 759.6124 761.3264 762.0613 763.6263 765.3916 766.1630 766.6383 768.1712 768.4751 770.9312 772.5539 774.4183 776.4239 777.9918 779.3284 782.1962 786.2209 788.4823 808.0707 812.2408 824.8008 833.9392 838.7457 842.6120 843.4796 859.0344 870.3268 874.4834 877.1987 878.0193 886.3201 894.5600 913.8594
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		916.7738 920.2063 947.1909 1029.6370 1031.4478 1034.0129 1039.3427 1041.3054 1044.2456 1052.3392 1061.4785 1064.1776 1080.4386 1138.8952 1145.3580 1145.9671 1149.4246 1152.1652 1158.0440 1170.8120 1176.6951 1182.7373 1192.1451 1193.9384 1201.3458 1205.4552 1212.3450 1237.2204 1238.3323 1242.7130 1246.2683 1255.8840 1258.7028 1272.8083 1274.3908 1277.0708 1279.5179 1286.1394 1288.0165 1289.3793 1291.9444 1298.0114 1304.0714 1312.5027 1317.7599 1319.2182 1333.9751 1343.0118 1345.0332 1349.0639
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		1355.0636 1357.9638 1361.8274 1365.2451 1367.5877 1368.4134 1371.3309 1380.7919 1382.9403 1385.4208 1386.5433 1389.4619 1392.1723 1394.9156 1397.6171 1400.3839 1402.2675 1403.7897 1408.5000 1416.8684 1424.0420 1425.5438 1428.1412 1429.5938 1432.4455 1435.9365 1441.3631 1452.1988 1461.8653 1473.5883 1477.7710 1484.3371 1485.4003 1489.1516 1491.3410 1501.6207 1505.6326 1516.8485 1529.4911 1536.1337 1540.9916 1542.9652 1554.3328 1555.9737 1560.7070 1576.0892 1586.6365 1590.4723 1591.2741 1592.5816
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					1601.4705 1603.9647 1610.1438 1611.2087 1615.9222 1621.1419 1626.8680 1633.8816 1657.0151 1665.3940 1672.3087 1675.4702 1691.7222 1694.7846 1704.8279 1711.0887 1717.5013 1722.0434 1849.8492 2006.6717 2950.1418 3736.8211 3746.9068
CW_WM @C84	C	-2.52776800	-1.78361200	-2.86794000	64.5441
	C	-3.17241400	-2.19637000	-1.66993700	76.5716
	C	-2.54525600	-3.24778400	-0.97315400	86.3889
	C	-1.23441300	-2.24621600	-3.21041600	161.6154
	C	-0.54006400	-3.20450300	-2.43513800	163.2406
	C	-1.27540300	-3.75937500	-1.35829800	174.0317
	C	-3.95637500	-1.21161900	-0.90788900	182.0619
	C	-4.04050000	-1.34118300	0.50361500	220.3777
	C	-2.62840400	-0.41156500	-3.33707800	221.4305
	C	-3.35656400	0.50454700	-2.63423900	225.0400
	C	-4.05405600	0.10929500	-1.41157600	227.9253
	C	-1.36370200	-0.01831700	-3.91556100	239.4091
	C	-0.84473900	1.29406200	-3.72368400	269.1849
	C	0.55541800	1.40652300	-3.76974200	278.2259
	C	0.87794600	-1.05444800	-3.76414400	281.2310
	C	-0.51795900	-1.16008000	-3.86993700	287.8212
	C	1.39365800	0.26653200	-3.84981900	289.4401
	C	1.63648300	-2.08375000	-3.03559500	295.4352
	C	1.54659700	-3.76794400	-1.23679700	299.1091
	C	0.92772900	-3.16578800	-2.36064600	301.8440
	C	2.90021900	-1.71504000	-2.53541300	308.0499
	C	-3.39305900	2.32224800	-1.22596300	321.7911
	C	-4.06871400	1.22807300	-0.54064000	331.3107
	C	-3.99674500	1.10155700	0.87243500	335.6584
	C	-4.06413600	-0.22230500	1.37504300	337.8582
	C	-2.70940900	3.26125000	-0.50216700	344.5948

C	-1.59921700	2.26944400	-2.93123500	349.5196
C	-2.87147000	1.86638800	-2.47564100	362.5744
C	-1.48451000	3.79431400	-1.00735300	367.2268
C	-0.87487100	3.28932800	-2.16743800	369.4732
C	-2.63887400	3.17235000	0.94900700	377.9786
C	-3.24812300	2.10767900	1.64216300	379.3646
C	-2.60515000	1.71432900	2.84732100	383.5029
C	-2.67161000	0.33742000	3.31250900	386.1236
C	-3.37074400	-0.59824400	2.60618100	391.7165
C	0.64630900	4.23475200	0.11159000	392.9337
C	-0.71219400	4.18508100	0.15284200	396.1715
C	-1.38677900	3.71625200	1.34363900	406.6457
C	-0.64757600	3.18041200	2.42469900	421.3250
C	-1.32589200	2.20902000	3.19629400	448.5766
C	1.27753300	2.45620000	-3.04501700	449.1045
C	0.59268700	3.37567600	-2.22533100	452.7722
C	1.33402400	3.88307400	-1.11567500	457.0100
C	-2.62870700	-3.34081700	0.47751000	461.1770
C	-3.34006200	-2.41516900	1.19356700	463.9444
C	-2.84246500	-1.94486800	2.44826000	471.6388
C	-1.40160100	-0.02217300	3.90434400	475.1779
C	0.55692800	-1.39497300	3.77457000	477.1197
C	-0.84494600	-1.31960600	3.71719900	478.5901
C	-1.56547200	-2.31497300	2.91750200	486.2379
C	-0.80802000	-3.31827000	2.16125000	491.3950
C	-1.39573200	-3.84106000	0.99448800	497.4987
C	1.42990100	3.80608300	1.25240200	497.8980
C	0.81817200	3.18287500	2.36271700	498.3385
C	1.54687300	2.12133500	3.04242300	501.1810
C	0.81227700	1.07355300	3.76456700	504.2059
C	-0.58627400	1.14076900	3.86107500	508.4172
C	1.36247900	-0.23265000	3.85788700	509.7074
C	1.31341100	-2.42117800	3.05410000	514.3287
C	0.66307100	-3.36475000	2.23311900	515.2580
C	1.43199000	-3.85243600	1.13048100	516.3511
C	0.76216000	-4.21751700	-0.10317200	521.4475
C	-0.59919500	-4.20597600	-0.15915600	525.1132
C	3.33072000	0.42913700	2.62078300	529.3360
C	2.63002200	-0.55055100	3.25294900	533.0506
C	2.58926500	-1.89934800	2.72576900	536.1885
C	3.26958800	-2.24028100	1.52675900	537.3451
C	2.69668200	-3.29354400	0.77640200	541.4666
C	2.67425700	3.35077200	0.71382100	544.2184
C	3.35883800	2.35638300	1.36531600	546.4279
C	2.82591900	1.78851300	2.56168400	547.0068
C	2.56421500	1.96746600	-2.70582700	559.7175
C	3.21899700	2.32267600	-1.49580200	575.6575
C	2.60755200	3.35720300	-0.74907400	584.9853
C	4.07083600	-0.02617200	-1.36029000	592.1319
C	3.36966900	-0.34243600	-2.59119900	594.3260

C	2.64635000	0.61768200	-3.22962400	597.2702
C	4.05272600	1.31316800	0.61542100	604.9705
C	3.97910300	1.27228400	-0.79440800	607.3570
C	2.77583600	-3.28290400	-0.68634000	616.2712
C	4.05371100	0.12904200	1.39749000	616.5798
C	4.01012800	-1.17134800	0.83114400	628.9819
C	4.10225200	-1.20994100	-0.57786100	632.9149
C	3.43867300	-2.26837000	-1.33311400	636.8209
C	-1.11004900	0.05664300	0.00921200	637.5941
O	-1.11108200	-0.01562200	-1.15172200	643.7986
O	-1.13398500	0.02488800	1.16743000	654.4597
H	0.72065900	-1.46189000	-0.78924400	659.0268
O	0.85204000	1.40284100	0.02134700	659.5181
H	0.95897700	1.34511500	-0.93633700	663.4716
H	0.62610400	-1.65668500	0.74270000	666.1882
H	1.20389400	0.54690400	0.31765400	669.0474
O	1.10282900	-1.17774100	0.05193200	669.5824
				673.0793
				675.5006
				681.7916
				687.5213
				693.7842
				695.0086
				695.8325
				700.3331
				701.6021
				702.8631
				712.7940
				719.2807
				719.6755
				720.9333
				721.8186
				728.5072
				730.6639
				734.2286
				735.9109
				741.6403
				745.1981
				746.0702
				749.3262
				750.0780
				751.3476
				752.6703
				754.2591
				758.1951
				761.6031
				761.8598
				763.3548
				765.7201
				766.0633

		768.0512 768.9102 769.7700 770.5512 771.8895 772.5661 773.6474 775.3668 775.9724 777.5272 779.4421 786.9697 789.3140 807.3272 819.9671 824.2265 833.6532 838.3267 843.2794 857.3034 870.8519 873.8097 877.2781 884.5104 893.9342 913.3536 914.6154 920.5763 946.4663 1028.2619 1030.5364 1031.8022 1038.2853 1040.1636 1042.1811 1048.5466 1058.9919 1062.9326 1138.9691 1140.6483 1143.6843 1148.9736 1151.2498 1168.7859 1173.1787 1179.4949 1191.6064 1191.7983 1194.8964 1202.8604
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		1213.4469 1233.3827 1236.9738 1243.6541 1244.1071 1252.5185 1261.4882 1270.4959 1273.2264 1275.1850 1276.2479 1284.6676 1285.4862 1287.2972 1290.2810 1297.7670 1299.3045 1309.5398 1315.1534 1317.7424 1333.3424 1340.4919 1344.8268 1346.3039 1353.0301 1355.6895 1358.7658 1365.2752 1367.1786 1370.2990 1371.4581 1374.3985 1381.0920 1382.2262 1385.0354 1386.6281 1391.3460 1393.8849 1394.0803 1396.0884 1397.6631 1398.4977 1407.7308 1415.2557 1419.5225 1423.8356 1428.1563 1430.8395 1434.6661 1437.2419
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		1440.0284 1447.3379 1457.1895 1469.5010 1474.1302 1483.3289 1485.0351 1485.9950 1487.5958 1498.6113 1515.1193 1529.2419 1532.1937 1537.1539 1540.9288 1552.3777 1554.5223 1559.1942 1577.9035 1583.4917 1586.6101 1590.5095 1592.4097 1599.5751 1605.5846 1607.3816 1611.0279 1612.8889 1618.4407 1625.0178 1632.0134 1654.8785 1660.8897 1667.1282 1670.3549 1685.9225 1691.9358 1699.5516 1703.4243 1710.5211 1713.0889 1719.1862 2485.2907 3742.8682 3828.6415 3909.3966 3925.2871

Table S3: Absolute Energies (hartree) obtained at DLPNO-CCSD(T)/cc-pVTZ//M06-2X/6-31G** level of theory:

Species	Energies (hartree)
CA	-264.6510927077
TS	-264.579990145
CW	-264.6613799754
C60	-2281.8826454644
CA@C60	-2546.4727654895
TS@C60	-2546.4030795018
CW@C60	-2546.4272108122
C-70	-2662.2913583755
CA@C70	-2926.9582848478
TS@C70	-2926.8920316182
CW@C70	-2926.9386901374
C-84	-3194.8603842834
CA@C84	-3459.5573921454
TS@C84	-3459.4877625103
CW@C84	-3459.5535919491

Table S4: Absolute Energies (hartree) in presence of OEEF obtained at M06-2X/6-31G** level of theory:

	Field Free	X+003	X+006	X+009	X+012	X+024
CA	-264.90220	-264.90211	-264.90226	-264.90261	-264.90317	-264.90746
TS	-264.83088	-264.83406	-264.83748	-264.84114	-264.84502	-264.86289
CW	-264.90087	-264.89844	-264.89844	-264.89399	-264.89196	-264.89399
CA@C60	-2550.29297	-2550.29526	-2550.30183	-2550.31264	-2550.32769	-2550.43045
TS@C60	-2550.22295	-2550.22564	-2550.23289	-2550.24437	-2550.26010	-2550.36554
CW@C60	-2550.24438	-2550.24854	-2550.25669	-2550.26906	-2550.28567	-2550.39443
CA@C70	-2931.38288	-2931.38584	-2931.39425	-2931.40810	-2931.42742	-2931.55979
TS@C70	-2931.31450	-2931.31811	-2931.32715	-2931.34165	-2931.36159	-2931.49634
CW@C70	-2931.35424	-2931.35609	-2931.36394	-2931.37726	-2931.39606	-2931.52672
CA@C84	-3464.81805	-3464.82062	-3464.83035	-3464.84668	-3464.86960	-3465.02772
TS@C84	-3464.74660	-3464.74923	-3464.75844	-3464.77425	-3464.79667	-3464.95285
CW@C84	-3464.80615	-3464.80904	-3464.81866	-3464.83489	-3464.85775	-3465.01591

Table S5: Equilibrium constants in presence of OEEF along X axis for the uncatalyzed decomposition reaction of CA in gas phase:

OEEF(in au)	Keq
X+0.003	1.30E+07
X+0.006	1.12E+07
X+0.009	6.86E+04
X+0.012	4.43E+03
X+0.024	4.00E+02