Chemisorption of CO_2 by Diamine-Tetraamido Macrocyclic Motifs: A Theoretical Study

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Electronic Supplementary Information

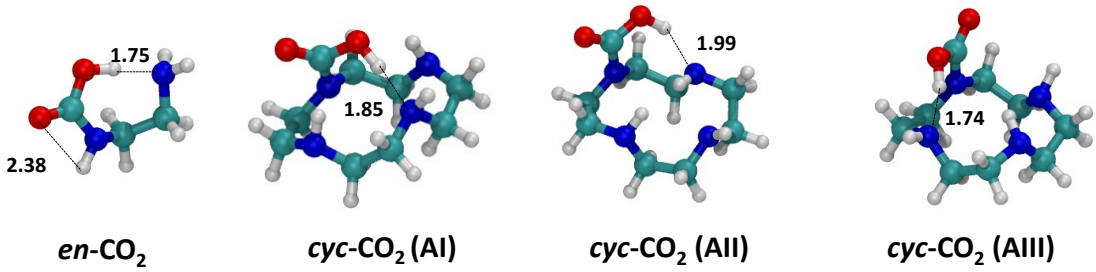

Figure S1. DFT-optimized structures of *en*-carbamated and *cyc*-carbamated adducts in gas phase at B3LYP/6-31G*; different protonation sites were simulated. Short intramolecular interactions are given in Å.

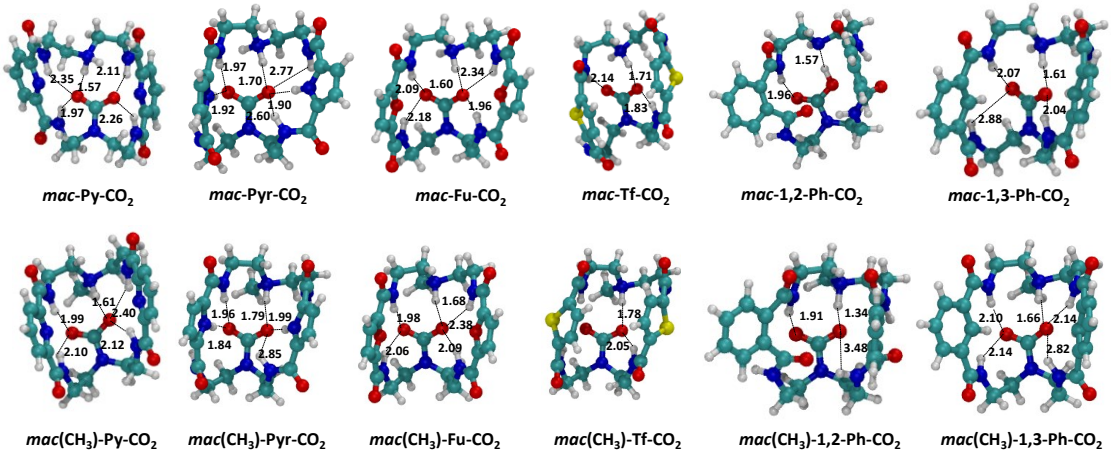

Figure S2. DFT-calculated structures (calculated at B3LYP/6-31G*) of *mac*-Z-CO_2 adducts in the gas phase. Short intramolecular interactions are given in Å.

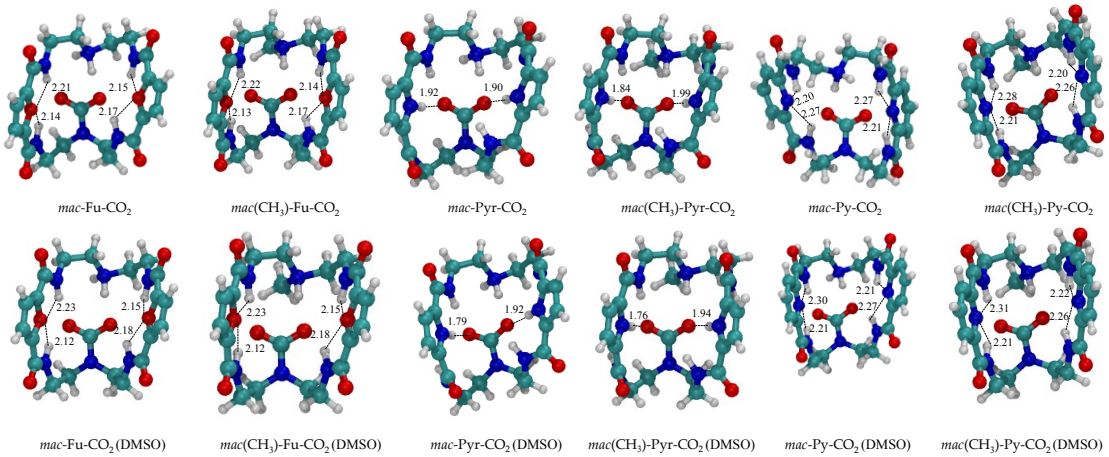

Figure S3. DFT-calculated structures in gas phase (top) and DMSO (bottom), at B3LYP/6-31G* for selected *mac*-Z-CO_2 adducts indicating intramolecular hydrogen bonding within the macrocyclic structure. Short intramolecular interactions are given in Å.

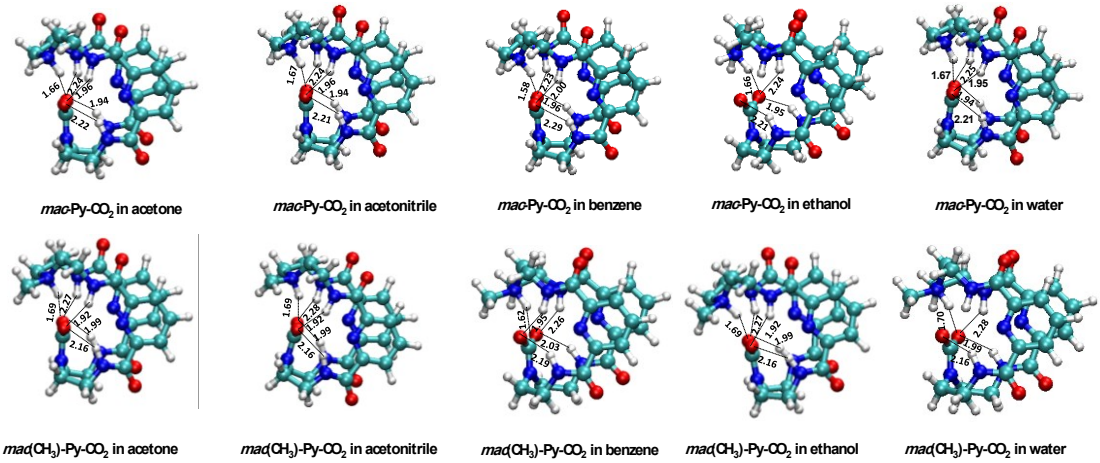

Figure S4. DFT-calculated structures (in DMSO at M06-2X/6-311++G**) of *mac*(CH_3)-Py-CO_2 adducts in different solvents. Short intramolecular interactions are given in Å.

Table S1. Thermodynamic parameters (in kcal/mol) for the chemical reaction of CO_2 with *cyc* in gas phase.

CO_2 adduct	**B3LYP/6-31G***		
	ΔH	**$T\Delta S$**	**ΔG**
***cyc*-CO_2 (AI)**	16.26	−11.26	27.52
***cyc*-CO_2 (AII)**	4.46	−11.37	15.83
***cyc*-CO_2 (AIII)**	7.19	−11.01	18.21

Table S2. Thermodynamic parameters (in kcal/mol) for the chemical reaction of CO_2 with *cyc* in DMSO.

CO_2 adduct	**B3LYP/6-31G***			**M06-2X/6-311++G****		
	ΔH	$T\Delta S$	ΔG	ΔH	$T\Delta S$	ΔG
***cyc*-CO_2 (BI)**	7.89	−11.29	19.18	1.74	−11.22	12.96
***cyc*-CO_2 (BII)**	−1.48	−10.92	9.44	−6.34	−11.00	4.66
***cyc*-CO_2 (BIII)**	1.53	−11.59	13.12	−7.89	−11.79	3.90

Table S3. Thermodynamic parameters (in kcal/mol) for the chemical reaction of CO_2 with *mac*-Py-CO_2 in different solvents (M06-2X/6-311++G**).

Solvent	**ΔH**	**$T\Delta S$**	**ΔG**
Water	−26.28	−14.82	−11.46
Ethanol	−26.37	−14.93	−11.44
Acetone	−26.38	−15.00	−11.38
Benzene	−26.20	−15.19	−11.00
Acetonitrile	−26.34	−14.86	−11.48

Table S4. Thermodynamic parameters (in kcal/mol) for the chemical reaction of CO_2 with *mac*(CH_3)-Py-CO_2 in different solvents (M06-2X/6-311++G**).

Solvent	**ΔH**	**$T\Delta S$**	**ΔG**
Water	−27.09	−14.08	−13.02
Ethanol	−27.05	−14.49	−12.56
Acetone	−27.04	−14.51	−12.54
Benzene	−26.15	−15.91	−10.23
Acetonitrile	−27.07	−14.34	−12.73

Table S5. Intramolecular hydrogen bond distances (in Å) of different *mac*-Z-CO_2 molecules as labelled in Scheme 3 (in gas phase at B3LYP/6-31G*).

mac-Z-CO_2	H-N_1-**H--O**-C	C-N_2-**H--O**-C	C-N_3-**H--O**-C	C-N_4-**H--O**-C	C-N_5-**H--O**-C
mac-Py-CO_2	1.57	2.35	1.97	2.26	2.11
mac-Pyr-CO_2	1.70	2.77	2.60	2.87	1.97
mac-Fu-CO_2	1.60	2.34	1.96	2.18	2.09
mac-Tf-CO_2	1.71	3.14	1.83	3.70	2.14
mac-1,2-Ph-CO_2	1.04	3.16	3.43	3.30	1.96
mac-1,3-Ph-CO_2	1.61	3.00	2.04	2.88	2.07

Table S6. Distances (in Å) between the nitrogen atoms in the carbamate group (O_2C–**N**) and the ammonium group (–**N**HR) as well as the **M----M** atoms in the cycle rings of *mac*-Z and *mac*-Z-CO_2 adducts; as defined in Scheme 3 (in gas phase at B3LYP/6-31G*).

mac-Z	H_2**N----N**H_2	**M----M**	***mac*-Z-CO_2**	**CO_2-N----NH_2**	**M----M**
mac-Py	4.58	8.04	*mac*-Py-CO_2	4.48	6.07
mac-Pyr	6.63	5.43	*mac*-Pyr-CO_2	4.63	5.65
mac-Fu	5.93	5.54	*mac*-Fu-CO_2	4.55	6.06
mac-Tf	7.95	4.88	*mac*-Tf -CO_2	4.58	6.94
mac-1,2-Ph	3.32	4.59[a]	*mac*-1,2-Ph -CO_2	4.71	5.88[a]
mac-1,3-Ph	5.99	5.72	*mac*-1,3-Ph -CO_2	4.53	5.97
mac(CH_3)-Z	H_2**N----N**H	**M----M**	*mac*(CH_3)-Z-CO_2	CO_2-**N----N**H	**M----M**
mac(CH_3)-Py	5.49	6.57	*mac*(CH_3)-Py-CO_2	4.63	5.52
mac(CH_3)-Pyr	6.74	5.11	*mac*(CH_3)-Pyr-CO_2	4.80	5.20
mac(CH_3)-Fu	6.46	5.38	*mac*(CH_3)-Fu-CO_2	4.70	5.59
mac(CH_3)-Tf	8.27	4.91	*mac*(CH_3)-Tf -CO_2	4.83	7.02
mac(CH_3)-1,2-Ph	3.58	4.45[a]	*mac*(CH_3)- 1,2-Ph -CO_2	4.63	5.79[a]
mac(CH_3)-1,3-Ph	6.16	5.47	*mac*(CH_3)- 1,3-Ph -CO_2	4.72	5.88

[a] Values are presented as an average of distances between C_1---C_1 and C_2---C_2, for the mac-1,2-Ph, due the lack of a central atom.

Table S7. Intramolecular hydrogen bond distances (in Å) of *mac*-Py-CO_2 molecule in different solvents (calculated at M06-2X/6-311++G**).

Solvent	**H-N_1-H--O-C**	**C-N_2-H--O-C**	**C-N_3-H--O-C**	**C-N_4-H--O-C**	**C-N_5-H--O-C**
DMSO	1.67	2.25	1.94	2.21	1.96
Water	1.67	2.25	1.94	2.21	1.96
Ethanol	1.66	2.24	1.95	2.21	1.96
Benzene	1.58	2.23	1.96	2.29	2.00
Acetonitrile	1.67	2.24	1.94	2.21	1.96
Acetone	1.66	2.24	1.95	2.22	1.96

Ethylenediamine (gas)

E(RB3LYP) = -190.524305790 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.577111	-0.494206	0.089635
2	1	0	-0.470733	-0.982612	1.071846
3	1	0	-0.496019	-1.282002	-0.671563
4	6	0	0.577098	0.494225	-0.089597
5	1	0	0.470689	0.982650	-1.071796
6	1	0	0.496041	1.282007	0.671622
7	7	0	1.864869	-0.183201	0.113414
8	1	0	2.055962	-0.827897	-0.652214
9	1	0	2.629203	0.488267	0.129999
10	7	0	-1.864859	0.183167	-0.113446
11	1	0	-2.629207	-0.488287	-0.129962
12	1	0	-2.055930	0.828002	0.652071

Ethylenediamine-CO_2 (gas)

E(RB3LYP) = -379.121396106 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.946319	-0.430436	-0.259119
2	1	0	-2.896726	-0.824689	0.130864
3	1	0	-1.890234	-0.678377	-1.323567
4	6	0	-0.779256	-1.111818	0.467126
5	1	0	-0.731111	-0.749754	1.505671
6	1	0	-0.983695	-2.186462	0.515655
7	7	0	0.513802	-0.955112	-0.202164
8	1	0	1.025266	-1.811558	-0.372669
9	6	0	1.400655	0.109198	-0.032099
10	8	0	2.600212	-0.031050	-0.186397
11	8	0	0.848264	1.291033	0.287447
12	1	0	-2.309891	1.520361	-0.895880
13	1	0	-2.308355	1.357425	0.734006
14	1	0	-0.139331	1.303961	0.113212
15	7	0	-1.857261	1.039050	-0.122284

Ethylenediamine (DMSO)

E(RB3LYP) = -190.534446961

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.578717	0.519680	-0.073874
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3	1	0	-0.469500	1.268740	0.721927
4	6	0	0.565229	-0.498643	0.025401
5	1	0	0.451116	-1.074908	0.960084
6	1	0	0.485144	-1.212103	-0.804627
7	7	0	1.871091	0.174462	-0.082383
8	1	0	2.042397	0.734504	0.752792
9	1	0	2.618372	-0.517579	-0.112132
10	7	0	-1.932254	-0.045737	0.025425
11	1	0	-2.041736	-0.544032	0.908446
12	1	0	-2.077239	-0.737566	-0.709736

Ethylenediamine-CO_2 (DMSO)

E(RB3LYP) = 379.127578283 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.571973	-0.045238	0.553955
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3	1	0	1.151876	0.884977	0.936159
4	6	0	0.657903	-0.645922	-0.519354
5	1	0	0.623821	0.025559	-1.387333
6	1	0	1.056807	-1.611221	-0.849391
7	7	0	-0.670413	-0.853097	0.020482
8	1	0	-1.037230	-1.794480	-0.019683
9	6	0	-1.651799	0.169247	0.003182
10	8	0	-2.839154	-0.203717	0.245395
11	8	0	-1.242486	1.345816	-0.224703
12	1	0	3.544031	0.703922	0.695554
13	1	0	3.410916	-0.533845	-0.386868
14	1	0	2.863176	0.973946	-0.781988
15	7	0	2.931660	0.294141	-0.016942

Cyclen (gas)

E(RB3LYP) = -535.880302752 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.119304	1.775036	-0.516441
2	7	0	-1.748974	1.167075	-0.537726
3	6	0	-1.119304	1.917075	0.545878
4	6	0	0.100406	2.685056	0.022556
5	6	0	2.001582	1.145082	0.470349
6	6	0	-2.669718	0.112298	-0.119431
7	1	0	1.675388	2.250204	-1.223058
8	1	0	-1.009536	0.746063	-1.099799
9	1	0	-1.841020	2.638310	0.954841
10	1	0	-0.802850	1.279478	1.393376
11	1	0	-0.227819	3.338075	-0.794418
12	1	0	0.493438	3.330908	0.829059
13	1	0	1.392522	0.863223	1.335851
14	1	0	2.778372	1.837769	0.847175
15	1	0	-3.268252	-0.182160	-0.993919
16	1	0	-3.374773	0.526662	0.613946
17	6	0	2.669718	-0.112298	-0.119431
18	6	0	-2.001582	-1.145082	0.470349
19	7	0	1.748974	-1.167075	-0.537726
20	1	0	3.268252	0.182160	-0.993919
21	1	0	3.374773	-0.526662	0.613946
22	7	0	-1.119304	-1.775036	-0.516441
23	1	0	-1.392522	-0.863223	1.335851
24	1	0	-2.778372	-1.837769	0.847175
25	6	0	1.119304	-1.917075	0.545878
26	1	0	1.009536	-0.746063	-1.099799
27	6	0	-0.100406	-2.685056	0.022556
28	1	0	-1.675388	-2.250204	-1.223058
29	1	0	1.841020	-2.638310	0.954841
30	1	0	0.802850	-1.279478	1.393376
31	1	0	0.227819	-3.338075	-0.794418
32	1	0	-0.493438	-3.330908	0.829059

Cyclen-CO_2 A11 (gas)

E(RB3LYP) = -724.462025978 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	6	0	2.671057	-0.759423	0.077095
4	6	0	2.092958	-2.152267	-0.209818
5	6	0	-0.018570	-2.129434	1.097302
6	6	0	2.351865	1.605615	-0.546298
7	1	0	0.244651	-2.854098	-0.807575
8	1	0	1.225856	-0.011598	-1.133381
9	1	0	3.767910	-0.816404	0.034365
10	1	0	2.418668	-0.473042	1.116909
11	1	0	2.417068	-2.463415	-1.209193
12	1	0	2.515958	-2.871041	0.516485
13	1	0	0.555558	-1.468998	1.757847
14	1	0	-0.020172	-3.123883	1.583966
15	1	0	2.258017	2.217632	-1.454474
16	1	0	3.374929	1.754036	-0.175730
17	6	0	-1.469906	-1.628496	1.004649
18	6	0	1.361200	2.134153	0.510614
19	7	0	-1.553604	-0.290554	0.415220
20	1	0	-2.066268	-2.298541	0.382524
21	1	0	-1.920442	-1.622860	2.007331
22	1	0	1.296479	1.419599	1.336475
23	1	0	1.730674	3.080348	0.940565
24	6	0	-1.391266	0.800287	1.387632
25	6	0	-1.114531	2.229103	0.897110
26	1	0	-2.291806	0.859269	2.022702
27	1	0	-0.573859	0.501265	2.054522
28	1	0	-1.999139	2.630656	0.394157
29	1	0	-0.947619	2.840629	1.799936
30	6	0	-2.015365	-0.223650	-0.898492
31	8	0	-2.592973	-1.147830	-1.446016
32	8	0	-1.753821	0.920825	-1.561884
33	1	0	-0.031975	3.214357	-0.529541
34	1	0	-0.954253	1.368743	-1.160515
35	7	0	0.007281	2.313526	-0.054881

Cyclen-CO_2 B11 (DMSO)

E(RB3LYP) = -724.483721179 A.U.

Number of Imaginary frequencies = 0

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	7	0	-1.619965	1.570652	0.239516
2	7	0	1.222348	1.579461	0.861405
3	6	0	0.674477	2.415756	-0.206815
4	6	0	-0.789345	2.771562	0.093065
5	6	0	-2.151106	0.985666	-0.994349
6	6	0	2.561214	1.036520	0.655344
7	1	0	-2.372055	1.738148	0.900953
8	1	0	0.548793	0.851967	1.100023
9	1	0	1.260445	3.342614	-0.270219
10	1	0	0.733244	1.946079	-1.205662
11	1	0	-0.826957	3.317255	1.042646
12	1	0	-1.156708	3.453354	-0.693854
13	1	0	-1.449019	1.205944	-1.805288
14	1	0	-3.112917	1.434680	-1.297280
15	1	0	2.913928	0.620194	1.607546
16	1	0	3.236179	1.866212	0.409874
17	6	0	-2.353740	-0.542462	-0.871709
18	6	0	2.751645	-0.026429	-0.445816
19	7	0	-1.160676	-1.254923	-0.399938
20	1	0	-3.157104	-0.757074	-0.167170
21	1	0	-2.649273	-0.938185	-1.853501
22	1	0	2.339700	0.309320	-1.398868
23	1	0	3.817258	-0.215207	-0.598437
24	6	0	-0.052345	-1.153099	-1.359018
25	6	0	1.216961	-1.970619	-1.138313
26	1	0	-0.455844	-1.488392	-2.322652
27	1	0	0.240339	-0.106705	-1.514063
28	1	0	0.994583	-2.985132	-0.800360
29	1	0	1.774443	-2.024620	-2.076438
30	6	0	-1.041318	-1.435875	0.998444
31	8	0	-2.096182	-1.519562	1.672625
32	8	0	0.139053	-1.551384	1.506047
33	1	0	2.832254	-2.019053	0.165212
34	1	0	1.406408	-1.296606	0.732720
35	7	0	2.106962	-1.348524	-0.096633

Cyclen-CO_2 A1 (gas)

E(RB3LYP) = -724.466514800 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.517559	0.282636	-0.874951

2	7	0	0.215296	2.097846	-0.418278
3	6	0	1.327637	1.973091	0.512012
4	6	0	2.612152	1.609865	-0.244994
5	6	0	2.936784	-0.872454	-0.068138
6	6	0	-1.119907	2.304755	0.127785
7	1	0	2.989866	0.278706	-1.773509
8	1	0	0.225058	1.323587	-1.077222
9	1	0	1.475706	2.938543	1.016848
10	1	0	1.162459	1.225515	1.311561
11	1	0	2.758383	2.350051	-1.039487
12	1	0	3.473814	1.681358	0.440143
13	1	0	2.886293	-0.587232	0.988652
14	1	0	3.982543	-1.162796	-0.262812
15	1	0	-1.797404	2.452913	-0.716223
16	1	0	-1.118252	3.238474	0.708524
17	6	0	2.007035	-2.076642	-0.325726
18	6	0	-1.713110	1.207623	1.048168
19	1	0	2.113317	-2.399179	-1.369219
20	1	0	2.294289	-2.926280	0.305868
21	7	0	-1.652947	-0.155913	0.499013
22	1	0	-1.164191	1.180487	1.994752
23	1	0	-2.753588	1.482725	1.274372
24	6	0	0.204559	-1.633699	1.314081
25	6	0	-1.283425	-1.261699	1.395059
26	1	0	0.358445	-2.601730	1.807639
27	1	0	0.804455	-0.889165	1.863529
28	1	0	-1.894314	-2.133510	1.142630
29	1	0	-1.541563	-0.979511	2.422362
30	6	0	-2.321567	-0.414752	-0.689106
31	8	0	-3.071422	0.380798	-1.225454
32	8	0	-2.069733	-1.629650	-1.244798
33	1	0	-1.200401	-1.989689	-0.937611
34	1	0	0.473787	-0.824877	-0.516037
35	7	0	0.591463	-1.750869	-0.096869

Cyclen-CO_2 B1 (DMSO)

E(RB3LYP) = -724.489896605 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.346083	0.417375	-0.838572
2	7	0	-0.001659	2.188617	-0.411728
3	6	0	1.120498	2.102727	0.523358
4	6	0	2.409774	1.764664	-0.233814

5	6	0	2.963296	-0.677381	-0.078796
6	6	0	-1.345597	2.280566	0.160954
7	1	0	2.717280	0.434218	-1.784071
8	1	0	0.036399	1.391052	-1.044088
9	1	0	1.241206	3.073578	1.022444
10	1	0	0.969309	1.356675	1.324490
11	1	0	2.541081	2.491443	-1.042671
12	1	0	3.272696	1.862426	0.440511
13	1	0	2.944941	-0.419130	0.984645
14	1	0	4.014612	-0.850505	-0.345979
15	1	0	-2.036322	2.420577	-0.673174
16	1	0	-1.395983	3.182267	0.787112
17	6	0	2.178225	-1.977198	-0.317474
18	6	0	-1.850166	1.095668	1.023434
19	1	0	2.272524	-2.303206	-1.355932
20	1	0	2.501835	-2.786716	0.339639
21	7	0	-1.592185	-0.238782	0.469590
22	1	0	-1.359927	1.127116	2.001178
23	1	0	-2.926389	1.251677	1.198904
24	6	0	0.275529	-1.661184	1.348038
25	6	0	-1.219124	-1.305960	1.399072
26	1	0	0.467163	-2.642890	1.788145
27	1	0	0.887051	-0.919040	1.864293
28	1	0	-1.804004	-2.199314	1.167891
29	1	0	-1.458307	-1.008078	2.424997
30	6	0	-2.170259	-0.642999	-0.768991
31	8	0	-2.904798	0.185509	-1.369763
32	8	0	-1.852806	-1.814441	-1.169404
33	1	0	0.065299	-2.277457	-0.620036
34	1	0	0.584989	-0.743969	-0.471469
35	7	0	0.726664	-1.693308	-0.080458

Cyclen-CO_2 A111 (gas)

E(RB3LYP) = -724.447076639 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.865184	1.628430	-0.134422
2	6	0	0.637250	2.109347	-0.762311
3	6	0	-0.410644	2.545535	0.274860
4	6	0	-2.387953	1.179558	-0.226362
5	6	0	2.648190	0.621034	-0.838234
6	1	0	1.717628	1.353458	0.830294
7	1	0	0.877634	2.973200	-1.400128

8	1	0	0.185996	1.351058	-1.421344
9	1	0	0.106169	2.955061	1.151301
10	1	0	-1.020298	3.361382	-0.145751
11	1	0	-1.950929	1.172626	-1.229034
12	1	0	-3.123487	2.003059	-0.218242
13	1	0	3.507511	0.396559	-0.203121
14	1	0	3.039900	1.057411	-1.767608
15	6	0	-3.127705	-0.148673	0.019304
16	6	0	1.937254	-0.716182	-1.216084
17	7	0	-2.330138	-1.365674	0.014589
18	1	0	-3.646750	-0.108598	0.986243
19	1	0	-3.915741	-0.225800	-0.744606
20	7	0	0.895008	-1.107870	-0.264957
21	1	0	1.433954	-0.613553	-2.184938
22	1	0	2.707209	-1.496178	-1.331251
23	6	0	-1.461251	-1.635986	-1.131615
24	1	0	-1.836061	-1.491036	0.889751
25	6	0	-0.071150	-2.133300	-0.709202
26	1	0	-1.917100	-2.414030	-1.764860
27	1	0	-1.334691	-0.750908	-1.770826
28	1	0	-0.189990	-2.881498	0.084806
29	1	0	0.386284	-2.659515	-1.555978
30	6	0	1.196322	-1.006961	1.090639
31	8	0	0.103979	-0.766375	1.864535
32	8	0	2.319315	-1.063211	1.557997
33	1	0	-1.704665	1.712301	1.620704
34	1	0	-0.450035	-0.081404	1.376025
35	7	0	-1.290163	1.436095	0.729408

Cyclen-CO_2 B111 (DMSO)

E(RB3LYP) = -724.475771973 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.218502	1.353240	-0.110286
2	6	0	-1.245090	2.269984	0.491766
3	6	0	-0.147650	2.650491	-0.491582
4	6	0	2.130284	1.651199	0.036350
5	6	0	-2.707650	0.261691	0.728041
6	1	0	-1.895329	0.956790	-0.989400
7	1	0	-1.740640	3.199488	0.802993
8	1	0	-0.786204	1.849088	1.399249
9	1	0	-0.570378	2.902260	-1.467458
10	1	0	0.430453	3.505153	-0.137357

11	1	0	1.873725	1.785169	1.088898
12	1	0	2.604029	2.567767	-0.322501
13	1	0	-3.468007	-0.259925	0.147261
14	1	0	-3.204138	0.691866	1.608698
15	6	0	3.052929	0.437902	-0.198159
16	6	0	-1.670306	-0.763401	1.250063
17	7	0	2.469535	-0.878203	0.000969
18	1	0	3.442559	0.478205	-1.222289
19	1	0	3.913499	0.577604	0.469711
20	7	0	-0.545581	-1.121719	0.356669
21	1	0	-1.203846	-0.367355	2.158914
22	1	0	-2.225801	-1.666347	1.553301
23	6	0	1.811187	-1.148531	1.284893
24	1	0	1.861578	-1.161828	-0.770955
25	6	0	0.497261	-1.902255	1.076552
26	1	0	2.463963	-1.757103	1.929196
27	1	0	1.604812	-0.224339	1.844497
28	1	0	0.697411	-2.819271	0.514968
29	1	0	0.101873	-2.197851	2.054804
30	6	0	-0.818312	-1.566278	-0.993831
31	8	0	-1.996885	-1.450447	-1.421079
32	8	0	0.194251	-1.970682	-1.642084
33	1	0	1.020869	1.390366	-1.699714
34	1	0	0.373456	0.604356	-0.391133
35	7	0	0.824729	1.499559	-0.700343

Cyclen (DMSO)

E(RB3LYP) = -535.889863873 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.123035	1.767730	-0.521120
2	7	0	-1.752289	1.176625	-0.549860
3	6	0	-1.123035	1.943025	0.531427
4	6	0	0.111283	2.690789	0.014103
5	6	0	1.982070	1.127164	0.483278
6	6	0	-2.668217	0.119201	-0.103447
7	1	0	1.706449	2.258733	-1.195189
8	1	0	-1.001226	0.731804	-1.079373
9	1	0	-1.842164	2.676173	0.921334
10	1	0	-0.828501	1.310724	1.387193
11	1	0	-0.194884	3.354651	-0.802988
12	1	0	0.508220	3.327289	0.824867
13	1	0	1.355589	0.835795	1.332576

14	1	0	2.748392	1.817880	0.879829
15	1	0	-3.280362	-0.188429	-0.963192
16	1	0	-3.358406	0.539322	0.639635
17	6	0	2.668217	-0.119201	-0.103447
18	6	0	-1.982070	-1.127164	0.483278
19	7	0	1.752289	-1.176625	-0.549860
20	1	0	3.280362	0.188429	-0.963192
21	1	0	3.358406	-0.539322	0.639635
22	7	0	-1.123035	-1.767730	-0.521120
23	1	0	-1.355589	-0.835795	1.332576
24	1	0	-2.748392	-1.817880	0.879829
25	6	0	1.123035	-1.943025	0.531427
26	1	0	1.001226	-0.731804	-1.079373
27	6	0	-0.111283	-2.690789	0.014103
28	1	0	-1.706449	-2.258733	-1.195189
29	1	0	1.842164	-2.676173	0.921334
30	1	0	0.828501	-1.310724	1.387193
31	1	0	0.194884	-3.354651	-0.802988
32	1	0	-0.508220	-3.327289	0.824867

***mac*-Pyridine (gas)**

E(RB3LYP) = -1594.24976272 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.288056	3.484712	0.370338
2	8	0	-4.417900	-3.302800	-1.579922
3	8	0	4.009564	-3.540301	0.259419
4	8	0	4.755622	3.362186	-1.132617
5	7	0	0.185317	2.238779	0.466638
6	6	0	-0.418769	2.436527	1.786170
7	1	0	0.195304	3.145973	2.352590
8	1	0	-0.370828	1.483598	2.333765
9	6	0	-1.873675	2.932751	1.784703
10	1	0	-1.974610	3.889444	1.263885
11	1	0	-2.207673	3.090735	2.821247
12	7	0	-2.736034	1.974926	1.106587
13	1	0	-2.544662	0.981425	1.175598
14	6	0	-3.874642	2.328144	0.453739
15	6	0	-4.612287	1.181257	-0.203732
16	7	0	-4.015087	-0.019480	-0.230642
17	6	0	-5.865529	1.417701	-0.777415
18	1	0	-6.289755	2.414396	-0.727024
19	6	0	-6.518824	0.354985	-1.401171

20	1	0	-7.496428	0.499278	-1.853247
21	6	0	-5.895592	-0.891416	-1.448969
22	1	0	-6.343007	-1.749979	-1.937372
23	6	0	-4.637781	-1.031773	-0.852499
24	6	0	-3.921631	-2.364386	-0.953012
25	7	0	-2.723228	-2.412164	-0.327621
26	1	0	-2.382759	-1.573191	0.128256
27	6	0	-1.804259	-3.532239	-0.425688
28	1	0	-1.192316	-3.440411	-1.337418
29	1	0	-2.382289	-4.455399	-0.521767
30	6	0	-0.901511	-3.588081	0.807562
31	1	0	-1.509468	-3.824584	1.689647
32	1	0	-0.178503	-4.410791	0.671992
33	7	0	-0.273733	-2.281464	1.045613
34	6	0	0.539314	-2.198629	2.261839
35	1	0	0.586219	-1.146039	2.579332
36	1	0	0.018781	-2.738949	3.061040
37	6	0	1.974612	-2.736267	2.141523
38	1	0	1.996549	-3.754362	1.743518
39	1	0	2.441730	-2.762447	3.137860
40	7	0	2.750521	-1.895438	1.241537
41	1	0	2.680812	-0.886588	1.322319
42	6	0	3.727440	-2.352262	0.413085
43	6	0	4.467404	-1.259322	-0.331193
44	7	0	4.020507	-0.002456	-0.195714
45	6	0	5.581747	-1.585327	-1.109797
46	1	0	5.889712	-2.622361	-1.185963
47	6	0	6.260043	-0.551316	-1.756467
48	1	0	7.134725	-0.764641	-2.365035
49	6	0	5.803504	0.758889	-1.612951
50	1	0	6.291418	1.602168	-2.089290
51	6	0	4.668736	0.986479	-0.826773
52	6	0	4.131117	2.398417	-0.684502
53	7	0	2.937869	2.474617	-0.052267
54	1	0	2.491055	1.609587	0.231288
55	6	0	2.172936	3.689460	0.151116
56	1	0	2.599128	4.478028	-0.475191
57	1	0	2.261420	4.017087	1.197717
58	6	0	0.699997	3.439881	-0.209913
59	1	0	0.630363	3.269447	-1.289758
60	1	0	0.114030	4.346143	0.015192
61	1	0	0.302578	-2.022751	0.243407
62	1	0	-0.472398	1.752735	-0.137165

***mac*(CH_3)-Pyridine (gas)**

E(RB3LYP)= -1633.55596950 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.081215	2.956087	-2.684453
2	8	0	-3.844438	-3.190805	0.704062
3	8	0	3.033321	-3.979417	-1.539391
4	8	0	4.214269	2.813321	0.047408
5	7	0	-0.190692	3.285715	1.505658
6	6	0	-0.986928	4.136517	0.601487
7	1	0	-0.617652	5.178656	0.607578
8	1	0	-2.019508	4.163772	0.966246
9	6	0	-1.006460	3.610280	-0.835227
10	1	0	0.015652	3.466375	-1.209806
11	1	0	-1.502573	4.325692	-1.496009
12	7	0	-1.748046	2.361414	-0.921403
13	1	0	-1.547483	1.634465	-0.245228
14	6	0	-2.744996	2.149681	-1.814682
15	6	0	-3.451005	0.814226	-1.696117
16	7	0	-3.212923	0.051361	-0.619178
17	6	0	-4.324949	0.426190	-2.718340
18	1	0	-4.481880	1.096517	-3.555969
19	6	0	-4.957217	-0.812222	-2.620166
20	1	0	-5.636533	-1.147056	-3.399377
21	6	0	-4.702697	-1.617469	-1.510350
22	1	0	-5.155001	-2.594810	-1.383145
23	6	0	-3.828817	-1.138209	-0.530089
24	6	0	-3.535840	-1.999299	0.679327
25	7	0	-2.909444	-1.348611	1.696670
26	1	0	-2.703757	-0.368349	1.536567
27	6	0	-2.371231	-2.011202	2.876039
28	1	0	-2.598316	-3.075242	2.772557
29	1	0	-2.876077	-1.644696	3.780564
30	6	0	-0.854876	-1.756951	2.985869
31	1	0	-0.690098	-0.679064	3.131747
32	1	0	-0.465397	-2.256025	3.881292
33	7	0	-0.075899	-2.190922	1.826245
34	6	0	0.304137	-3.610140	1.804804
35	1	0	0.977985	-3.783077	2.653750
36	1	0	-0.549619	-4.300135	1.909283
37	6	0	1.024905	-3.938276	0.494418
38	1	0	0.302746	-3.985262	-0.335238
39	1	0	1.499197	-4.922995	0.554780
40	7	0	2.027065	-2.921580	0.219964
41	1	0	1.901460	-2.024018	0.676658
42	6	0	2.878299	-2.984041	-0.828643
43	6	0	3.647082	-1.705034	-1.091236
44	7	0	3.314397	-0.613012	-0.386750
45	6	0	4.646975	-1.697920	-2.069477
46	1	0	4.861700	-2.614607	-2.607664

47	6	0	5.325398	-0.505105	-2.316726
48	1	0	6.109171	-0.462938	-3.068314
49	6	0	4.983368	0.634129	-1.588625
50	1	0	5.474403	1.589560	-1.736197
51	6	0	3.967666	0.531450	-0.631997
52	6	0	3.596401	1.753868	0.177393
53	7	0	2.565856	1.592987	1.047215
54	1	0	2.133572	0.678726	1.091638
55	6	0	2.214892	2.633375	2.004129
56	1	0	3.140891	3.151085	2.273966
57	1	0	1.831790	2.145321	2.905158
58	6	0	1.225783	3.685393	1.477288
59	1	0	1.509353	3.918103	0.447394
60	1	0	1.365906	4.616468	2.062532
61	6	0	-0.723458	3.326760	2.868389
62	1	0	-0.154088	2.659227	3.522275
63	1	0	-0.689611	4.342315	3.309423
64	1	0	-1.763998	2.986449	2.870014
65	1	0	-0.598517	-1.965411	0.978767

***mac*-Pyridine-CO_2 (gas)**

E(RB3LYP) = -1782.85872352 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	5.004677	1.525865	0.711207
2	8	0	1.103698	-4.360485	1.049300
3	8	0	-4.687014	-2.026178	0.618251
4	8	0	-1.075895	3.856330	2.134205
5	8	0	0.590219	-0.141779	-1.833119
6	8	0	-1.329153	0.951949	-2.267798
7	7	0	1.208557	2.392228	-1.954507
8	1	0	0.929992	1.383497	-1.644986
9	6	0	2.524626	2.266672	-2.662500
10	1	0	2.708141	3.186349	-3.227399
11	1	0	2.402178	1.439748	-3.368158
12	6	0	3.694656	2.009274	-1.714993
13	1	0	3.911210	2.884989	-1.095011
14	1	0	4.587606	1.846794	-2.336735
15	7	0	3.449246	0.884174	-0.835468
16	1	0	2.801050	0.142135	-1.090971
17	6	0	4.155285	0.724537	0.321128
18	6	0	3.804205	-0.522550	1.094788
19	7	0	2.816800	-1.275496	0.596702

20	6	0	4.495478	-0.855104	2.262628
21	1	0	5.285279	-0.204476	2.622226
22	6	0	4.134842	-2.031874	2.923197
23	1	0	4.649391	-2.328657	3.833229
24	6	0	3.109850	-2.823217	2.403626
25	1	0	2.793604	-3.749282	2.871418
26	6	0	2.470106	-2.399482	1.232643
27	6	0	1.350022	-3.225471	0.630908
28	7	0	0.692780	-2.611321	-0.374610
29	1	0	0.960895	-1.665270	-0.644421
30	6	0	-0.348111	-3.253180	-1.160438
31	1	0	-1.308299	-3.232784	-0.627858
32	1	0	-0.076571	-4.307367	-1.292608
33	6	0	-0.487096	-2.582607	-2.538442
34	1	0	0.511431	-2.427502	-2.962995
35	1	0	-1.018432	-3.278367	-3.195989
36	7	0	-1.229576	-1.318006	-2.577399
37	6	0	-2.603734	-1.327054	-3.082454
38	1	0	-2.808607	-0.336367	-3.494967
39	1	0	-2.672543	-2.052993	-3.902025
40	6	0	-3.669886	-1.674212	-2.033508
41	1	0	-3.542239	-2.690515	-1.642638
42	1	0	-4.660459	-1.640202	-2.510388
43	7	0	-3.593540	-0.737213	-0.927002
44	1	0	-3.024897	0.097708	-1.045958
45	6	0	-4.034266	-1.023497	0.318968
46	6	0	-3.634478	-0.002225	1.363356
47	7	0	-2.809438	0.976121	0.973735
48	6	0	-4.094506	-0.118180	2.679325
49	1	0	-4.757222	-0.936953	2.937813
50	6	0	-3.670806	0.828441	3.612981
51	1	0	-4.007971	0.771058	4.644509
52	6	0	-2.804556	1.846766	3.211039
53	1	0	-2.439647	2.604802	3.895379
54	6	0	-2.399175	1.876361	1.872878
55	6	0	-1.460485	2.953832	1.387633
56	7	0	-1.088374	2.842426	0.080974
57	1	0	-1.457121	2.076265	-0.485031
58	6	0	-0.289582	3.859666	-0.560099
59	1	0	-0.236042	4.713344	0.122018
60	1	0	-0.789083	4.193340	-1.481067
61	6	0	1.146616	3.434655	-0.878040
62	1	0	1.641775	3.030520	0.006902
63	1	0	1.708914	4.306643	-1.231980
64	6	0	-0.645592	-0.114225	-2.214765
65	1	0	0.469748	2.573595	-2.644798

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mac(CH_3)-Pyridine-CO_2 (gas)

E(RB3LYP)= -1822.16579094 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.761878	0.015147	1.517596
2	8	0	0.252104	4.653838	-0.280505
3	8	0	4.772654	1.307412	0.546622
4	8	0	0.021041	-3.357419	2.920641
5	8	0	-0.620294	-0.236663	-2.023132
6	8	0	1.158382	-1.606140	-1.819561
7	7	0	-1.924963	-2.502269	-1.545929
8	1	0	-1.306756	-1.609929	-1.523262
9	6	0	-3.301303	-2.019817	-1.938502
10	1	0	-3.872295	-2.890018	-2.279607
11	1	0	-3.139647	-1.354794	-2.791862
12	6	0	-4.093030	-1.305330	-0.848267
13	1	0	-4.378068	-1.982056	-0.037258
14	1	0	-5.037071	-0.980105	-1.311761
15	7	0	-3.374395	-0.180684	-0.286382
16	1	0	-2.617152	0.271046	-0.794751
17	6	0	-3.813518	0.430180	0.851468
18	6	0	-3.042515	1.671439	1.225187
19	7	0	-2.073022	2.045396	0.382464
20	6	0	-3.360634	2.389563	2.380745
21	1	0	-4.157192	2.038155	3.027612
22	6	0	-2.630528	3.548964	2.652097
23	1	0	-2.845619	4.136155	3.540872
24	6	0	-1.627257	3.949670	1.769153
25	1	0	-1.038037	4.847125	1.923422
26	6	0	-1.379720	3.158825	0.641046
27	6	0	-0.311973	3.559100	-0.355636
28	7	0	-0.063875	2.633982	-1.307104
29	1	0	-0.563664	1.747465	-1.280360
30	6	0	0.881401	2.853435	-2.388717
31	1	0	1.887414	3.013972	-1.982173
32	1	0	0.608853	3.769597	-2.930738
33	6	0	0.861122	1.668583	-3.363516
34	1	0	-0.169086	1.483220	-3.684181
35	1	0	1.437822	1.952001	-4.251524
36	7	0	1.419705	0.416456	-2.851830
37	6	0	2.825793	0.107001	-3.126810
38	1	0	2.910098	-0.975158	-3.258940
39	1	0	3.102311	0.583315	-4.074958
40	6	0	3.822690	0.562836	-2.050428
41	1	0	3.819339	1.652405	-1.928763
42	1	0	4.837268	0.283828	-2.371514
43	7	0	3.495640	-0.056504	-0.779234

44	1	0	2.778261	-0.780032	-0.774188
45	6	0	3.938916	0.408413	0.409353
46	6	0	3.298980	-0.264874	1.606405
47	7	0	2.326241	-1.147934	1.356599
48	6	0	3.702953	0.058789	2.906049
49	1	0	4.495123	0.785863	3.048859
50	6	0	3.058740	-0.569644	3.972941
51	1	0	3.346055	-0.344328	4.996634
52	6	0	2.038206	-1.486868	3.714351
53	1	0	1.501782	-1.999566	4.505278
54	6	0	1.706680	-1.743076	2.379829
55	6	0	0.612316	-2.726180	2.040521
56	7	0	0.348511	-2.853736	0.710206
57	1	0	0.871319	-2.298909	0.027094
58	6	0	-0.600177	-3.830377	0.229498
59	1	0	-0.834623	-4.492216	1.069220
60	1	0	-0.139613	-4.441254	-0.554306
61	6	0	-1.939173	-3.243042	-0.231235
62	1	0	-2.296980	-2.545485	0.526833
63	1	0	-2.671878	-4.051699	-0.345036
64	6	0	-1.359390	-3.322829	-2.663049
65	1	0	-0.283578	-3.412221	-2.520672
66	1	0	-1.850340	-4.299917	-2.681835
67	1	0	-1.541576	-2.794117	-3.600206
68	6	0	0.627182	-0.522211	-2.201272

***mac*-Pyridine (DMSO)**

E(RB3LYP) = -1594.27718632 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.793591	-2.162439	1.228217
2	8	0	-3.279779	-2.394044	1.415097
3	8	0	-3.841128	1.876919	0.906781
4	8	0	3.126016	3.140902	0.909912
5	7	0	2.671333	0.121841	-2.536342
6	6	0	3.138977	-1.233728	-2.832823
7	1	0	3.978769	-1.167055	-3.535021
8	1	0	2.328556	-1.754311	-3.359575
9	6	0	3.591272	-2.094103	-1.637054
10	1	0	4.436972	-1.642866	-1.113400
11	1	0	3.920132	-3.074306	-2.009845
12	7	0	2.515036	-2.258535	-0.667104
13	1	0	1.566681	-2.403784	-0.996739

14	6	0	2.690721	-2.264377	0.670329
15	6	0	1.420877	-2.388146	1.487131
16	7	0	0.248512	-2.368766	0.836482
17	6	0	1.510184	-2.496609	2.879240
18	1	0	2.484124	-2.507367	3.354409
19	6	0	0.330340	-2.585164	3.616963
20	1	0	0.362582	-2.673649	4.698796
21	6	0	-0.891456	-2.551669	2.946006
22	1	0	-1.836372	-2.607409	3.473825
23	6	0	-0.883860	-2.439331	1.551544
24	6	0	-2.199745	-2.375104	0.805375
25	7	0	-2.099580	-2.280891	-0.535070
26	1	0	-1.165051	-2.345069	-0.923257
27	6	0	-3.257541	-2.216883	-1.421696
28	1	0	-3.979596	-1.517124	-0.993416
29	1	0	-3.747774	-3.200195	-1.464430
30	6	0	-2.846729	-1.816217	-2.849857
31	1	0	-2.156768	-2.583703	-3.228688
32	1	0	-3.742360	-1.868516	-3.479228
33	7	0	-2.221575	-0.513621	-3.067708
34	6	0	-3.058074	0.679806	-3.163984
35	1	0	-2.469563	1.452572	-3.678293
36	1	0	-3.902989	0.446637	-3.822294
37	6	0	-3.630961	1.300074	-1.876520
38	1	0	-4.265011	0.596892	-1.331441
39	1	0	-4.263744	2.155216	-2.156023
40	7	0	-2.565828	1.741278	-0.982262
41	1	0	-1.649113	1.953814	-1.359815
42	6	0	-2.752372	2.003605	0.326327
43	6	0	-1.520341	2.461234	1.078839
44	7	0	-0.355414	2.501043	0.415741
45	6	0	-1.633473	2.811323	2.428660
46	1	0	-2.600579	2.762059	2.915359
47	6	0	-0.485425	3.212975	3.110319
48	1	0	-0.536850	3.494440	4.157874
49	6	0	0.730787	3.241878	2.429136
50	1	0	1.653330	3.535374	2.916303
51	6	0	0.748324	2.875765	1.079043
52	6	0	2.064005	2.874406	0.328422
53	7	0	1.976124	2.563431	-0.981733
54	1	0	1.046135	2.381993	-1.340244
55	6	0	3.125158	2.458742	-1.876711
56	1	0	3.905040	3.128034	-1.504502
57	1	0	2.808727	2.804420	-2.865634
58	6	0	3.676750	1.031437	-1.978964
59	1	0	4.047727	0.720094	-0.988610
60	1	0	4.537129	1.047575	-2.659838
61	1	0	-1.416311	-0.368419	-2.464660
62	1	0	1.881812	0.064020	-1.894052

***mac*-Pyridine-CO_2 (DMSO)**

E(RB3LYP)= -1782.90179635 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	4.698444	1.676780	1.104567
2	8	0	1.065988	-4.390928	1.230139
3	8	0	-4.540312	-1.981719	0.957562
4	8	0	-1.221962	4.253592	1.417804
5	8	0	0.693141	-0.326350	-1.930987
6	8	0	-1.356897	0.570366	-2.201479
7	7	0	1.390375	2.265844	-2.306754
8	1	0	1.014201	1.328218	-1.961222
9	6	0	2.824177	2.050033	-2.722280
10	1	0	3.121855	2.890842	-3.352660
11	1	0	2.822586	1.142194	-3.330245
12	6	0	3.795726	1.933211	-1.553835
13	1	0	3.881822	2.876719	-1.008585
14	1	0	4.785351	1.728984	-1.984108
15	7	0	3.414343	0.890119	-0.614718
16	1	0	2.822438	0.117138	-0.910290
17	6	0	3.923212	0.830852	0.637906
18	6	0	3.474513	-0.363298	1.447229
19	7	0	2.657026	-1.229114	0.837693
20	6	0	3.918405	-0.540856	2.761228
21	1	0	4.580292	0.189235	3.212803
22	6	0	3.487934	-1.673386	3.454505
23	1	0	3.809649	-1.845739	4.477284
24	6	0	2.642794	-2.583187	2.817741
25	1	0	2.289539	-3.479674	3.314480
26	6	0	2.249011	-2.316471	1.501695
27	6	0	1.342984	-3.274267	0.758454
28	7	0	0.893360	-2.820693	-0.422525
29	1	0	1.144724	-1.877100	-0.722480
30	6	0	0.070517	-3.611933	-1.327813
31	1	0	-0.875088	-3.880701	-0.841480
32	1	0	0.589344	-4.549930	-1.566123
33	6	0	-0.184850	-2.842381	-2.629928
34	1	0	0.772306	-2.520089	-3.051844
35	1	0	-0.639808	-3.536448	-3.343054
36	7	0	-1.066200	-1.677503	-2.514430
37	6	0	-2.481150	-1.826843	-2.868211
38	1	0	-2.805328	-0.918347	-3.382999
39	1	0	-2.574457	-2.658965	-3.572904

40	6	0	-3.419294	-2.098909	-1.683461
41	1	0	-3.155035	-3.033667	-1.175095
42	1	0	-4.443680	-2.215751	-2.063616
43	7	0	-3.351151	-0.998197	-0.733026
44	1	0	-2.788107	-0.186588	-0.994184
45	6	0	-3.864669	-1.040301	0.507011
46	6	0	-3.542747	0.173125	1.354123
47	7	0	-2.747758	1.097082	0.801585
48	6	0	-4.046238	0.295269	2.653107
49	1	0	-4.687501	-0.478927	3.059015
50	6	0	-3.697103	1.426125	3.393446
51	1	0	-4.067965	1.555258	4.405991
52	6	0	-2.864420	2.387991	2.819802
53	1	0	-2.566048	3.280054	3.358449
54	6	0	-2.412647	2.178180	1.511633
55	6	0	-1.517384	3.195381	0.840562
56	7	0	-1.093356	2.867342	-0.401798
57	1	0	-1.371468	1.973319	-0.819499
58	6	0	-0.313788	3.783587	-1.213492
59	1	0	-0.352141	4.765345	-0.736406
60	1	0	-0.780404	3.876518	-2.201902
61	6	0	1.164054	3.410437	-1.359059
62	1	0	1.589682	3.132160	-0.394194
63	1	0	1.713433	4.266297	-1.760496
64	6	0	-0.559968	-0.418776	-2.206401
65	1	0	0.851706	2.440048	-3.161440

***mac*-Pyridine(CH_3) (DMSO)**

E(RB3LYP) = -1633.58428526 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.889274	-3.260522	-2.579690
2	8	0	4.394070	-1.049586	-0.189819
3	8	0	2.992923	2.648489	-0.945573
4	8	0	-4.081873	2.363522	-0.927891
5	7	0	-2.971603	-1.215307	1.916858
6	6	0	-3.178941	-2.599446	1.464232
7	1	0	-4.183871	-2.969662	1.740341
8	1	0	-2.454807	-3.234226	1.987266
9	6	0	-2.995327	-2.800339	-0.039246
10	1	0	-3.694292	-2.187232	-0.620562
11	1	0	-3.219472	-3.844924	-0.283195
12	7	0	-1.627162	-2.503748	-0.449020

13	1	0	-1.008531	-2.033869	0.202143
14	6	0	-1.179705	-2.758891	-1.692047
15	6	0	0.263315	-2.401163	-1.970906
16	7	0	1.048704	-2.066929	-0.936531
17	6	0	0.725119	-2.437438	-3.291962
18	1	0	0.045830	-2.719325	-4.087995
19	6	0	2.055047	-2.104416	-3.542536
20	1	0	2.445272	-2.115886	-4.555877
21	6	0	2.877511	-1.760280	-2.470856
22	1	0	3.920171	-1.499092	-2.609162
23	6	0	2.331282	-1.759753	-1.182991
24	6	0	3.222509	-1.415152	-0.008984
25	7	0	2.652348	-1.537613	1.207022
26	1	0	1.709109	-1.911665	1.228466
27	6	0	3.362316	-1.299938	2.457997
28	1	0	4.159348	-0.580900	2.257573
29	1	0	3.843878	-2.227616	2.801067
30	6	0	2.418381	-0.804325	3.568952
31	1	0	1.693818	-1.598441	3.792710
32	1	0	3.023571	-0.673646	4.474582
33	7	0	1.654197	0.420540	3.349328
34	6	0	2.370077	1.693107	3.245950
35	1	0	1.713623	2.487210	3.630789
36	1	0	3.232682	1.653330	3.920195
37	6	0	2.870766	2.133247	1.859563
38	1	0	3.549891	1.399556	1.416805
39	1	0	3.431220	3.072041	1.970084
40	7	0	1.749967	2.335375	0.944697
41	1	0	0.801755	2.360789	1.302680
42	6	0	1.895008	2.567944	-0.374478
43	6	0	0.599733	2.724762	-1.141819
44	7	0	-0.538185	2.420111	-0.502756
45	6	0	0.624741	3.169460	-2.467702
46	1	0	1.573132	3.398579	-2.939971
47	6	0	-0.587366	3.307361	-3.144104
48	1	0	-0.606746	3.654499	-4.172882
49	6	0	-1.773964	2.989843	-2.482927
50	1	0	-2.739754	3.074586	-2.967517
51	6	0	-1.699897	2.543252	-1.159348
52	6	0	-2.967011	2.162833	-0.421998
53	7	0	-2.770179	1.605384	0.789652
54	1	0	-1.807859	1.465136	1.072413
55	6	0	-3.838017	1.146153	1.665227
56	1	0	-4.750008	1.681307	1.389312
57	1	0	-3.583650	1.435131	2.689292
58	6	0	-4.112644	-0.360716	1.560084
59	1	0	-4.398288	-0.575039	0.526838
60	1	0	-4.991680	-0.592247	2.193684
61	6	0	-2.704021	-1.186794	3.358202
62	1	0	-2.487930	-0.167320	3.688556

63	1	0	-3.556251	-1.567075	3.953159
64	1	0	-1.826438	-1.801513	3.580069
65	1	0	0.979434	0.301735	2.598363

***mac*-Pyridine(CH_3)-CO_2 (DMSO)**

E(RB3LYP) = -1822.20741958 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.606931	0.054971	1.779994
2	8	0	0.487179	4.669510	0.112612
3	8	0	4.835378	1.024138	0.585187
4	8	0	-0.004784	-3.770701	2.504495
5	8	0	-0.692344	0.056860	-1.981451
6	8	0	1.051373	-1.372221	-1.932315
7	7	0	-2.140962	-2.245798	-1.736948
8	1	0	-1.482968	-1.417630	-1.622518
9	6	0	-3.510282	-1.651611	-1.993913
10	1	0	-4.144858	-2.449772	-2.387258
11	1	0	-3.362154	-0.910032	-2.782524
12	6	0	-4.201495	-1.024861	-0.788931
13	1	0	-4.462503	-1.771057	-0.034843
14	1	0	-5.151047	-0.615036	-1.159748
15	7	0	-3.403496	0.017098	-0.161961
16	1	0	-2.667532	0.488847	-0.682572
17	6	0	-3.699522	0.503175	1.065696
18	6	0	-2.836152	1.658181	1.515256
19	7	0	-1.922613	2.100332	0.643911
20	6	0	-3.018041	2.234458	2.776284
21	1	0	-3.771820	1.840283	3.448330
22	6	0	-2.211113	3.317793	3.127900
23	1	0	-2.321517	3.791824	4.098679
24	6	0	-1.264659	3.788078	2.216514
25	1	0	-0.622421	4.631450	2.443341
26	6	0	-1.153758	3.142246	0.980187
27	6	0	-0.151837	3.615695	-0.050466
28	7	0	-0.030896	2.818995	-1.124770
29	1	0	-0.573903	1.955575	-1.163924
30	6	0	0.841294	3.117930	-2.252495
31	1	0	1.867322	3.271131	-1.898228
32	1	0	0.521450	4.053980	-2.730409
33	6	0	0.780156	1.986868	-3.286201
34	1	0	-0.258899	1.831624	-3.591279
35	1	0	1.338314	2.310005	-4.170672

36	7	0	1.333070	0.705716	-2.843105
37	6	0	2.728054	0.389732	-3.163767
38	1	0	2.791025	-0.672027	-3.417095
39	1	0	3.014705	0.960652	-4.052457
40	6	0	3.738572	0.705114	-2.050529
41	1	0	3.748194	1.775727	-1.815211
42	1	0	4.745370	0.442572	-2.404145
43	7	0	3.407569	-0.047077	-0.848449
44	1	0	2.642424	-0.721729	-0.913751
45	6	0	3.929819	0.201445	0.363458
46	6	0	3.307608	-0.604429	1.485111
47	7	0	2.290937	-1.409207	1.153550
48	6	0	3.772390	-0.483876	2.798629
49	1	0	4.599568	0.180895	3.020516
50	6	0	3.142066	-1.233043	3.793851
51	1	0	3.474389	-1.164865	4.825564
52	6	0	2.078749	-2.068708	3.449682
53	1	0	1.558872	-2.666217	4.189662
54	6	0	1.686948	-2.124291	2.106900
55	6	0	0.547253	-3.022949	1.681588
56	7	0	0.204024	-2.951316	0.374710
57	1	0	0.699624	-2.307783	-0.251932
58	6	0	-0.799687	-3.828056	-0.202224
59	1	0	-1.024833	-4.599609	0.537846
60	1	0	-0.382578	-4.331436	-1.078892
61	6	0	-2.132768	-3.145716	-0.523879
62	1	0	-2.435765	-2.538374	0.328977
63	1	0	-2.894722	-3.909986	-0.705273
64	6	0	-1.679943	-2.949836	-2.979737
65	1	0	-0.611972	-3.142126	-2.901318
66	1	0	-2.241560	-3.878732	-3.095255
67	1	0	-1.861457	-2.293655	-3.831469
68	6	0	0.531157	-0.251035	-2.227063

***mac*-1,3-Ph (gas)**

E(RB3LYP) = -1562.14542680 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	4.388482	0.000408	-0.820008
2	8	0	-0.845093	4.889388	-1.228501
3	8	0	-5.147305	-1.302654	-0.388700
4	8	0	1.451378	-3.953579	-1.427545
5	6	0	3.465926	-0.830761	2.969580

6	1	0	4.128108	-1.414225	3.623572
7	1	0	2.910458	-0.143982	3.624206
8	6	0	4.351119	-0.011796	2.006680
9	1	0	4.933958	-0.665705	1.354826
10	1	0	5.059183	0.592250	2.592190
11	7	0	3.568760	0.855599	1.132043
12	1	0	3.141412	1.674634	1.544401
13	6	0	3.668154	0.808438	-0.237955
14	6	0	2.828703	1.797610	-1.001271
15	6	0	3.264369	2.172049	-2.279995
16	1	0	4.179185	1.733966	-2.666314
17	6	0	2.529354	3.090323	-3.029974
18	1	0	2.880099	3.388729	-4.014180
19	6	0	1.342836	3.623176	-2.524317
20	1	0	0.762016	4.342445	-3.092934
21	6	0	0.870899	3.226785	-1.265522
22	6	0	-0.432667	3.815081	-0.791786
23	7	0	-1.116538	3.092327	0.147602
24	1	0	-0.833577	2.142295	0.346186
25	6	0	-2.413819	3.497314	0.665912
26	1	0	-3.218474	2.994969	0.111403
27	1	0	-2.515956	4.570620	0.486693
28	6	0	-2.521121	3.198769	2.164283
29	1	0	-1.738347	3.766889	2.680766
30	1	0	-3.490854	3.572973	2.530880
31	7	0	-2.352629	1.768152	2.490442
32	6	0	-3.588215	1.027020	2.796731
33	1	0	-3.309517	0.158119	3.404576
34	1	0	-4.291263	1.635556	3.391432
35	6	0	-4.318424	0.529104	1.548904
36	1	0	-4.680533	1.370633	0.940605
37	1	0	-5.201765	-0.046189	1.840756
38	7	0	-3.446873	-0.336072	0.769661
39	1	0	-2.466290	-0.085900	0.764182
40	6	0	-3.939494	-1.191967	-0.176939
41	6	0	-2.930881	-2.012793	-0.935329
42	6	0	-3.299438	-2.488573	-2.201228
43	1	0	-4.287047	-2.245365	-2.580223
44	6	0	-1.149962	-3.574962	-2.432281
45	1	0	-0.440703	-4.167921	-3.000725
46	6	0	-0.777719	-3.138456	-1.152977
47	6	0	0.583528	-3.554795	-0.652805
48	7	0	0.799261	-3.468970	0.697419
49	1	0	0.009770	-3.307416	1.305454
50	6	0	2.040256	-3.931198	1.319799
51	1	0	2.471287	-4.704866	0.677249
52	1	0	1.778371	-4.372896	2.286821
53	6	0	3.064391	-2.811781	1.534466
54	1	0	3.431410	-2.456001	0.560081
55	1	0	3.921300	-3.241792	2.070122

56	6	0	-2.405989	-3.255723	-2.948860
57	1	0	-2.690444	-3.609181	-3.936275
58	6	0	-1.671189	-2.346173	-0.417705
59	1	0	-1.396399	-1.989445	0.571424
60	6	0	1.627731	2.323725	-0.505935
61	1	0	1.278068	2.023584	0.478452
62	7	0	2.497821	-1.742421	2.367003
63	1	0	1.838591	-1.206518	1.805020
64	1	0	-1.720420	1.678431	3.279333

***mac*-1,3-Ph-CO_2 (gas)**

E(RB3LYP)= -1750.75183453 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.817250	-1.407252	0.791880
2	8	0	-0.902622	4.584326	0.803700
3	8	0	4.392014	2.042453	0.512131
4	8	0	0.734332	-3.790384	2.353037
5	8	0	-0.485527	0.146278	-1.554898
6	8	0	1.206086	-1.195230	-2.189853
7	7	0	-1.501783	-2.301217	-1.754114
8	1	0	-1.174231	-1.310391	-1.454224
9	6	0	-2.706402	-2.164228	-2.638093
10	1	0	-2.855398	-3.113920	-3.163296
11	1	0	-2.449324	-1.399234	-3.377698
12	6	0	-3.986631	-1.789885	-1.881413
13	1	0	-4.300822	-2.579443	-1.194360
14	1	0	-4.785346	-1.683369	-2.629739
15	7	0	-3.827496	-0.587087	-1.094511
16	1	0	-3.485105	0.245263	-1.555703
17	6	0	-4.220743	-0.492631	0.226420
18	6	0	-3.815061	0.774103	0.915172
19	6	0	-4.529483	1.245179	2.024769
20	1	0	-5.397609	0.693794	2.373302
21	6	0	-4.116780	2.418904	2.661390
22	1	0	-4.679582	2.794578	3.511763
23	6	0	-2.985759	3.113629	2.218969
24	1	0	-2.665556	4.030735	2.704431
25	6	0	-2.241906	2.624779	1.138327
26	6	0	-1.024466	3.368869	0.640774
27	7	0	-0.114871	2.592345	-0.011883
28	1	0	-0.312855	1.606119	-0.136565
29	6	0	0.926067	3.112616	-0.886119

30	1	0	1.916855	2.977198	-0.435095
31	1	0	0.754983	4.188975	-0.990373
32	6	0	0.868767	2.445082	-2.276517
33	1	0	-0.170988	2.430145	-2.622026
34	1	0	1.438675	3.071999	-2.970962
35	7	0	1.432714	1.088361	-2.381981
36	6	0	2.711083	0.945445	-3.079825
37	1	0	2.786408	-0.093037	-3.410853
38	1	0	2.699810	1.579313	-3.978213
39	6	0	3.953141	1.312667	-2.245857
40	1	0	3.915325	2.341193	-1.877173
41	1	0	4.840177	1.229594	-2.890145
42	7	0	4.070791	0.440977	-1.089629
43	1	0	3.841712	-0.531635	-1.245387
44	6	0	4.096730	0.887913	0.204868
45	6	0	3.685064	-0.134413	1.229423
46	6	0	4.190880	-0.097930	2.534695
47	1	0	4.926409	0.656540	2.797751
48	6	0	2.761558	-1.966665	3.140533
49	1	0	2.393447	-2.680031	3.871091
50	6	0	2.230667	-1.993787	1.843793
51	6	0	1.159559	-2.995513	1.513896
52	7	0	0.679273	-2.974249	0.225644
53	1	0	1.063082	-2.346179	-0.478984
54	6	0	-0.314910	-3.918796	-0.228523
55	1	0	-0.499400	-4.622399	0.588128
56	1	0	0.074273	-4.491802	-1.084203
57	6	0	-1.648256	-3.273700	-0.611732
58	1	0	-2.089026	-2.735804	0.229822
59	1	0	-2.345335	-4.056009	-0.930659
60	6	0	0.698215	-0.040064	-2.038220
61	6	0	3.736377	-1.023213	3.478124
62	1	0	4.136582	-1.003115	4.488291
63	6	0	2.706831	-1.077193	0.902188
64	1	0	2.290036	-1.054586	-0.096624
65	6	0	-2.676721	1.466354	0.489249
66	1	0	-2.104903	1.083624	-0.346496
67	1	0	-0.695887	-2.568706	-2.336209

***mac*(CH_3)-1,3-Ph (gas)**

E(RB3LYP) = -1601.45549951 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	8	0	-1.895143	-3.970992	-2.030458
2	8	0	4.676852	-2.221143	-0.115356
3	8	0	2.634823	3.792068	-1.339073
4	8	0	-4.353376	2.730553	-0.613943
5	7	0	-3.206287	-1.224111	2.043076
6	6	0	-3.395206	-2.644082	1.690551
7	1	0	-4.403364	-2.993653	1.982438
8	1	0	-2.673551	-3.232272	2.268457
9	6	0	-3.174959	-2.947172	0.209567
10	1	0	-3.873081	-2.388520	-0.428940
11	1	0	-3.368675	-4.007274	0.023470
12	7	0	-1.796249	-2.671084	-0.170147
13	1	0	-1.363891	-1.865322	0.263012
14	6	0	-1.254447	-3.209086	-1.305750
15	6	0	0.175194	-2.854351	-1.616722
16	6	0	0.596025	-2.982042	-2.947973
17	1	0	-0.128684	-3.294884	-3.692937
18	6	0	1.924321	-2.733194	-3.293811
19	1	0	2.242304	-2.831884	-4.328189
20	6	0	2.850226	-2.377718	-2.312856
21	1	0	3.894642	-2.214625	-2.559838
22	6	0	2.445327	-2.241025	-0.977906
23	6	0	3.498439	-1.903042	0.041354
24	7	0	3.075750	-1.236888	1.161335
25	1	0	2.201106	-0.727667	1.130160
26	6	0	4.033046	-0.785408	2.160852
27	1	0	4.774762	-0.112874	1.708464
28	1	0	4.591165	-1.649727	2.535517
29	6	0	3.308526	-0.105924	3.322356
30	1	0	2.652825	-0.838197	3.808894
31	1	0	4.066178	0.203442	4.063033
32	7	0	2.464101	1.023726	2.898316
33	6	0	3.180120	2.273812	2.567413
34	1	0	2.615429	3.114149	2.988202
35	1	0	4.180978	2.290341	3.027483
36	6	0	3.322334	2.502205	1.059457
37	1	0	3.963050	1.735574	0.602449
38	1	0	3.795362	3.469505	0.868904
39	7	0	2.009286	2.510924	0.433567
40	1	0	1.359833	1.814096	0.773987
41	6	0	1.768728	3.139336	-0.757051
42	6	0	0.375980	3.007410	-1.317171
43	6	0	0.198193	3.277245	-2.680974
44	1	0	1.066297	3.552868	-3.271216
45	6	0	-2.180017	2.880998	-2.469939
46	1	0	-3.178585	2.849034	-2.894406
47	6	0	-2.018755	2.599604	-1.106206
48	6	0	-3.249353	2.288578	-0.298548
49	7	0	-3.056958	1.500281	0.807542
50	1	0	-2.193062	0.981650	0.890561

51	6	0	-4.148074	1.087577	1.676004
52	1	0	-5.048639	1.592668	1.318738
53	1	0	-3.958437	1.441178	2.697541
54	6	0	-4.380616	-0.425949	1.649529
55	1	0	-4.658100	-0.706082	0.629441
56	1	0	-5.246042	-0.660302	2.300760
57	6	0	-2.919483	-1.089074	3.474125
58	1	0	-2.723981	-0.043861	3.730326
59	1	0	-3.752975	-1.445872	4.109113
60	1	0	-2.024965	-1.668056	3.724884
61	6	0	-1.072758	3.207761	-3.253033
62	1	0	-1.201861	3.419516	-4.311007
63	6	0	-0.739616	2.670809	-0.537114
64	1	0	-0.629251	2.536055	0.535812
65	6	0	1.105522	-2.478196	-0.636740
66	1	0	0.807892	-2.448013	0.408454
67	1	0	1.790392	1.210759	3.634762

***mac*(CH_3)-1,3-Ph-CO_2 (gas)**

E(RB3LYP) = -1790.05665985 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	4.323408	2.173023	1.597207
2	8	0	2.702280	-4.537117	0.209578
3	8	0	-3.726140	-3.201056	0.693118
4	8	0	-2.209714	3.681676	2.137952
5	8	0	0.759155	0.244901	-1.783340
6	8	0	-1.464324	0.516612	-2.005036
7	7	0	0.846091	2.936571	-1.787358
8	1	0	0.663204	1.892799	-1.590558
9	6	0	2.333233	3.037643	-2.051761
10	1	0	2.517210	4.014713	-2.510373
11	1	0	2.550776	2.259039	-2.788332
12	6	0	3.226692	2.876908	-0.826066
13	1	0	3.112440	3.706565	-0.121369
14	1	0	4.265506	2.932055	-1.183756
15	7	0	2.980530	1.620905	-0.145351
16	1	0	2.411221	0.922267	-0.611163
17	6	0	3.629659	1.328623	1.029999
18	6	0	3.453781	-0.064134	1.560209
19	6	0	3.936738	-0.383343	2.836381
20	1	0	4.402191	0.396166	3.431467
21	6	0	3.830325	-1.692093	3.316794

22	1	0	4.210034	-1.932351	4.306240
23	6	0	3.254744	-2.696915	2.533402
24	1	0	3.199054	-3.721206	2.890425
25	6	0	2.748628	-2.381088	1.267228
26	6	0	2.196932	-3.422630	0.330010
27	7	0	1.147112	-2.980827	-0.428187
28	1	0	0.738581	-2.085685	-0.193330
29	6	0	0.797234	-3.522151	-1.730906
30	1	0	-0.110152	-4.136303	-1.676972
31	1	0	1.613282	-4.180903	-2.045008
32	6	0	0.627129	-2.376976	-2.746230
33	1	0	1.517049	-1.744758	-2.732797
34	1	0	0.536521	-2.813965	-3.750715
35	7	0	-0.539611	-1.520188	-2.505841
36	6	0	-1.832674	-2.014568	-3.000789
37	1	0	-2.373291	-1.172525	-3.445063
38	1	0	-1.629793	-2.733849	-3.802714
39	6	0	-2.740050	-2.699744	-1.964517
40	1	0	-2.244775	-3.542124	-1.471919
41	1	0	-3.616863	-3.106555	-2.490727
42	7	0	-3.138114	-1.733941	-0.957689
43	1	0	-2.975966	-0.765687	-1.209711
44	6	0	-3.496962	-2.049828	0.319702
45	6	0	-3.586003	-0.861079	1.243056
46	6	0	-4.389568	-0.893494	2.388956
47	1	0	-4.938634	-1.800834	2.623024
48	6	0	-3.776397	1.405607	2.891384
49	1	0	-3.853771	2.292953	3.511892
50	6	0	-2.961585	1.441703	1.751324
51	6	0	-2.255214	2.712302	1.379479
52	7	0	-1.680037	2.743800	0.126026
53	1	0	-1.779886	1.965827	-0.524077
54	6	0	-1.068267	3.951399	-0.378280
55	1	0	-1.187508	4.713419	0.398272
56	1	0	-1.598483	4.312309	-1.268798
57	6	0	0.433389	3.830148	-0.638304
58	1	0	0.922824	3.439622	0.254877
59	1	0	0.841415	4.822626	-0.864882
60	6	0	0.098005	3.223250	-3.051574
61	1	0	-0.932322	2.889354	-2.938530
62	1	0	0.150138	4.292790	-3.271953
63	1	0	0.559514	2.650600	-3.857578
64	6	0	-0.415827	-0.193421	-2.084648
65	6	0	-4.475489	0.237066	3.208179
66	1	0	-5.102542	0.211363	4.095512
67	6	0	-2.857910	0.296600	0.960556
68	1	0	-2.183608	0.291206	0.115742
69	6	0	2.859144	-1.071033	0.794271
70	1	0	2.509398	-0.869998	-0.211282

***mac*-1,3-Ph (DMSO)**

E(RB3LYP) = -1562.18681826 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.646979	-1.649252	1.116775
2	8	0	-3.229288	-3.691066	1.247454
3	8	0	-3.787268	3.404333	0.577084
4	8	0	3.338257	2.597109	1.079846
5	6	0	3.495230	-1.280133	-2.832964
6	1	0	4.371767	-1.201528	-3.489189
7	1	0	2.694654	-1.740416	-3.426010
8	6	0	3.865116	-2.228493	-1.672524
9	1	0	4.659837	-1.808550	-1.054184
10	1	0	4.229537	-3.174732	-2.092364
11	7	0	2.733044	-2.504042	-0.792404
12	1	0	1.980900	-3.064757	-1.172585
13	6	0	2.699099	-2.192054	0.529137
14	6	0	1.434996	-2.540822	1.271319
15	6	0	1.529327	-2.797687	2.647022
16	1	0	2.500619	-2.745017	3.128209
17	6	0	0.389161	-3.126691	3.381236
18	1	0	0.471238	-3.337248	4.443782
19	6	0	-0.856473	-3.184921	2.754216
20	1	0	-1.747873	-3.441381	3.317623
21	6	0	-0.973349	-2.900407	1.386257
22	6	0	-2.342493	-2.969170	0.761846
23	7	0	-2.543602	-2.218544	-0.345464
24	1	0	-1.859260	-1.524214	-0.622035
25	6	0	-3.803704	-2.170591	-1.074794
26	1	0	-4.511484	-1.500599	-0.568809
27	1	0	-4.247202	-3.170086	-1.074730
28	6	0	-3.548105	-1.718672	-2.516877
29	1	0	-2.928690	-2.477102	-3.008193
30	1	0	-4.512879	-1.687234	-3.047534
31	7	0	-2.837157	-0.431819	-2.606164
32	6	0	-3.673436	0.770377	-2.757928
33	1	0	-3.109423	1.494946	-3.355499
34	1	0	-4.606056	0.550025	-3.301691
35	6	0	-4.039787	1.429356	-1.424852
36	1	0	-4.679909	0.771926	-0.821632
37	1	0	-4.605030	2.346325	-1.612235
38	7	0	-2.831009	1.773508	-0.686729

39	1	0	-2.051373	1.137093	-0.803550
40	6	0	-2.788836	2.733896	0.265986
41	6	0	-1.462162	2.972902	0.938413
42	6	0	-1.471302	3.525543	2.227336
43	1	0	-2.423201	3.750199	2.697415
44	6	0	0.946039	3.489532	2.275430
45	1	0	1.884539	3.679942	2.785323
46	6	0	0.976062	2.960995	0.976538
47	6	0	2.328620	2.694354	0.365744
48	7	0	2.389545	2.572613	-0.984581
49	1	0	1.566384	2.777652	-1.533099
50	6	0	3.643536	2.355447	-1.709237
51	1	0	4.432443	2.934400	-1.218846
52	1	0	3.500005	2.747533	-2.719773
53	6	0	4.065827	0.884472	-1.780059
54	1	0	4.284400	0.521942	-0.764255
55	1	0	5.001024	0.836003	-2.352503
56	6	0	-0.271521	3.773899	2.894567
57	1	0	-0.285054	4.191016	3.897500
58	6	0	-0.234678	2.697850	0.318812
59	1	0	-0.229757	2.282465	-0.684054
60	6	0	0.178918	-2.588285	0.650316
61	1	0	0.095858	-2.379874	-0.411982
62	7	0	3.063826	0.072702	-2.479116
63	1	0	2.218110	0.019986	-1.912371
64	1	0	-2.182604	-0.472826	-3.380425

***mac*-1,3-Ph-CO_2 (DMSO)**

E(RB3LYP) = -1750.79845007 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.442775	-1.505480	1.058591
2	8	0	-0.570978	4.508534	1.407631
3	8	0	4.669450	1.502053	1.091873
4	8	0	0.322348	-4.204740	1.488716
5	8	0	-0.435460	0.475128	-1.754524
6	8	0	1.433144	-0.704845	-2.210880
7	7	0	-1.849355	-1.871585	-2.271199
8	1	0	-1.338359	-1.021803	-1.886384
9	6	0	-3.194998	-1.468709	-2.836533
10	1	0	-3.490190	-2.246355	-3.545271
11	1	0	-3.023629	-0.542967	-3.391234
12	6	0	-4.306196	-1.299857	-1.797299
13	1	0	-4.502042	-2.226227	-1.255691
14	1	0	-5.218218	-1.052133	-2.353863

15	7	0	-4.010859	-0.269774	-0.817863
16	1	0	-3.863940	0.669617	-1.164728
17	6	0	-4.049535	-0.455235	0.534773
18	6	0	-3.512386	0.689938	1.342143
19	6	0	-3.974315	0.942865	2.641100
20	1	0	-4.761176	0.325074	3.063175
21	6	0	-3.423735	1.995896	3.376602
22	1	0	-3.789401	2.201554	4.378638
23	6	0	-2.404275	2.786527	2.835314
24	1	0	-1.977115	3.604093	3.407677
25	6	0	-1.916770	2.522484	1.548673
26	6	0	-0.824834	3.377538	0.956784
27	7	0	-0.175959	2.839891	-0.097472
28	1	0	-0.410966	1.903938	-0.425500
29	6	0	0.728606	3.572343	-0.974847
30	1	0	1.730164	3.643041	-0.532448
31	1	0	0.353834	4.594865	-1.101176
32	6	0	0.787453	2.880580	-2.346690
33	1	0	-0.231522	2.749136	-2.723755
34	1	0	1.311405	3.548408	-3.037025
35	7	0	1.475389	1.584007	-2.375401
36	6	0	2.871204	1.563150	-2.822966
37	1	0	3.043948	0.629237	-3.364651
38	1	0	3.021264	2.384870	-3.530875
39	6	0	3.918315	1.697801	-1.703196
40	1	0	3.780804	2.618734	-1.128730
41	1	0	4.917036	1.740233	-2.159800
42	7	0	3.805688	0.558006	-0.802823
43	1	0	3.315122	-0.240245	-1.193572
44	6	0	4.069537	0.573584	0.525443
45	6	0	3.569487	-0.635134	1.272738
46	6	0	4.201464	-1.083551	2.439895
47	1	0	5.062796	-0.546074	2.825197
48	6	0	2.631306	-2.933168	2.581812
49	1	0	2.275605	-3.832154	3.074715
50	6	0	1.987109	-2.486582	1.419014
51	6	0	0.845593	-3.281992	0.845232
52	7	0	0.448156	-2.957683	-0.418650
53	1	0	0.915634	-2.223694	-0.954891
54	6	0	-0.552380	-3.730834	-1.131701
55	1	0	-0.737385	-4.644872	-0.563209
56	1	0	-0.150495	-4.023828	-2.109618
57	6	0	-1.900279	-3.031724	-1.308445
58	1	0	-2.280421	-2.658790	-0.356831
59	1	0	-2.614030	-3.750109	-1.720314
60	6	0	0.797388	0.391847	-2.111919
61	6	0	3.726172	-2.227110	3.089940
62	1	0	4.221265	-2.579238	3.990590
63	6	0	2.452236	-1.326959	0.796369
64	1	0	1.932680	-0.942454	-0.070009

65	6	0	-2.486394	1.477881	0.813431
66	1	0	-2.116789	1.248515	-0.178011
67	1	0	-1.271764	-2.145096	-3.073788

***mac*(CH_3)-1,3-Ph (DMSO)**

E(RB3LYP) = -1601.49398803 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.703081	4.141683	-1.807745
2	8	0	-4.762836	1.871782	-0.381093
3	8	0	-2.723353	-2.380178	-1.385496
4	8	0	4.367789	-2.922131	-0.647193
5	7	0	3.156185	1.195166	2.022370
6	6	0	3.138668	2.665591	1.939325
7	1	0	4.067368	3.103682	2.347152
8	1	0	2.314366	3.025533	2.564523
9	6	0	2.932261	3.198126	0.521516
10	1	0	3.741133	2.888903	-0.152292
11	1	0	2.945739	4.292262	0.548458
12	7	0	1.644378	2.759473	-0.006091
13	1	0	1.248569	1.921541	0.403507
14	6	0	1.118468	3.268630	-1.144959
15	6	0	-0.226481	2.746471	-1.571470
16	6	0	-0.523428	2.724696	-2.941887
17	1	0	0.234015	3.040981	-3.652165
18	6	0	-1.780327	2.308591	-3.383446
19	1	0	-2.000502	2.283581	-4.446956
20	6	0	-2.759325	1.937966	-2.460295
21	1	0	-3.747999	1.638913	-2.794212
22	6	0	-2.476376	1.950906	-1.087128
23	6	0	-3.578769	1.593945	-0.127403
24	7	0	-3.208701	0.977759	1.018670
25	1	0	-2.284512	0.565037	1.100232
26	6	0	-4.165781	0.555947	2.033144
27	1	0	-4.809395	-0.243665	1.642628
28	1	0	-4.820992	1.396284	2.283391
29	6	0	-3.416011	0.099052	3.288337
30	1	0	-2.913136	0.965701	3.731673
31	1	0	-4.159570	-0.263054	4.018292
32	7	0	-2.382819	-0.904532	3.000217
33	6	0	-2.849661	-2.290535	2.855548
34	1	0	-2.110811	-2.952635	3.323869
35	1	0	-3.797884	-2.452367	3.394025

36	6	0	-3.062568	-2.741508	1.404686
37	1	0	-3.733171	-2.068390	0.868755
38	1	0	-3.535817	-3.733966	1.413274
39	7	0	-1.808362	-2.793170	0.660144
40	1	0	-0.993982	-3.141522	1.150152
41	6	0	-1.728749	-2.617506	-0.681631
42	6	0	-0.356423	-2.722072	-1.293055
43	6	0	-0.257598	-3.134684	-2.629340
44	1	0	-1.165116	-3.358345	-3.180988
45	6	0	2.155177	-2.984703	-2.515357
46	1	0	3.131900	-3.098661	-2.975216
47	6	0	2.070247	-2.534569	-1.190208
48	6	0	3.344867	-2.248108	-0.442827
49	7	0	3.302327	-1.231533	0.449103
50	1	0	2.472405	-0.654820	0.524695
51	6	0	4.415269	-0.860712	1.313782
52	1	0	5.346730	-1.162814	0.828847
53	1	0	4.351785	-1.411220	2.261392
54	6	0	4.439063	0.651601	1.548878
55	1	0	4.688198	1.140554	0.602848
56	1	0	5.254132	0.879204	2.261056
57	6	0	2.846775	0.750321	3.386414
58	1	0	2.784008	-0.340466	3.426646
59	1	0	3.606605	1.079373	4.119256
60	1	0	1.875462	1.152262	3.689088
61	6	0	0.993406	-3.270108	-3.234228
62	1	0	1.062564	-3.602849	-4.266025
63	6	0	0.812769	-2.410889	-0.584178
64	1	0	0.748446	-2.074065	0.446268
65	6	0	-1.205570	2.350350	-0.648494
66	1	0	-1.001447	2.414273	0.416615
67	1	0	-1.677019	-0.861433	3.728188

***mac*(CH_3)-1,3-Ph-CO_2 (DMSO)**

E(RB3LYP) = -1790.10383495 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.239918	-0.086867	1.699878
2	8	0	1.053407	4.591095	0.505939
3	8	0	4.807131	0.565985	0.929506
4	8	0	-0.922567	-3.558984	2.272336
5	8	0	-0.342713	0.249762	-1.885274
6	8	0	1.140462	-1.449408	-1.993726

7	7	0	-2.513688	-1.593804	-1.926161
8	1	0	-1.769440	-0.893070	-1.667966
9	6	0	-3.788148	-0.852886	-2.295150
10	1	0	-4.417832	-1.565933	-2.834496
11	1	0	-3.483445	-0.069811	-2.993603
12	6	0	-4.597795	-0.256903	-1.140040
13	1	0	-4.942371	-1.014323	-0.436026
14	1	0	-5.492074	0.186459	-1.595622
15	7	0	-3.859581	0.746519	-0.396108
16	1	0	-3.546227	1.559610	-0.910975
17	6	0	-3.695892	0.742652	0.959681
18	6	0	-2.749474	1.783907	1.480009
19	6	0	-2.888237	2.313307	2.770306
20	1	0	-3.714354	1.993397	3.398184
21	6	0	-1.966106	3.256468	3.231885
22	1	0	-2.079315	3.677968	4.226659
23	6	0	-0.895968	3.660285	2.426021
24	1	0	-0.178163	4.390582	2.786393
25	6	0	-0.733284	3.114757	1.145884
26	6	0	0.420817	3.545140	0.275690
27	7	0	0.695620	2.732464	-0.765341
28	1	0	0.174604	1.866984	-0.902037
29	6	0	1.649462	3.035834	-1.823850
30	1	0	2.676316	2.995326	-1.440470
31	1	0	1.478755	4.055474	-2.191667
32	6	0	1.451410	2.043598	-2.980156
33	1	0	0.412136	2.092804	-3.318013
34	1	0	2.085422	2.362962	-3.813141
35	7	0	1.777655	0.646668	-2.673175
36	6	0	3.120082	0.167517	-3.013387
37	1	0	3.043634	-0.877363	-3.326879
38	1	0	3.485155	0.741325	-3.871534
39	6	0	4.162682	0.280203	-1.885671
40	1	0	4.275535	1.311614	-1.539497
41	1	0	5.137066	-0.045135	-2.276256
42	7	0	3.748460	-0.550306	-0.761887
43	1	0	3.066419	-1.263972	-0.998144
44	6	0	3.987412	-0.284282	0.544736
45	6	0	3.167262	-1.101120	1.509254
46	6	0	3.627264	-1.384038	2.801928
47	1	0	4.592607	-1.005070	3.124131
48	6	0	1.608888	-2.666356	3.241200
49	1	0	1.011009	-3.284780	3.902910
50	6	0	1.136516	-2.381375	1.951914
51	6	0	-0.165765	-2.973178	1.482435
52	7	0	-0.446921	-2.860691	0.152369
53	1	0	0.203761	-2.413023	-0.497684
54	6	0	-1.601138	-3.508360	-0.445431
55	1	0	-2.000112	-4.217627	0.283859
56	1	0	-1.279190	-4.084770	-1.317380

57	6	0	-2.757696	-2.569493	-0.792442
58	1	0	-3.023815	-1.980089	0.085258
59	1	0	-3.622147	-3.170090	-1.091177
60	6	0	-1.977435	-2.261880	-3.162597
61	1	0	-0.944689	-2.556680	-2.984497
62	1	0	-2.601306	-3.123469	-3.405898
63	1	0	-2.003968	-1.538196	-3.977573
64	6	0	0.813272	-0.231831	-2.169410
65	6	0	2.843953	-2.161829	3.661020
66	1	0	3.203916	-2.387513	4.660953
67	6	0	1.915702	-1.581554	1.114455
68	1	0	1.542841	-1.315338	0.135967
69	6	0	-1.672518	2.186668	0.685655
70	1	0	-1.559553	1.741630	-0.294565

***mac*-1,2-Ph (gas)**

E(RB3LYP) = -1562.16091070 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.396526	1.028046	-2.597394
2	8	0	2.561051	2.361608	1.201014
3	8	0	-1.533962	-0.184667	2.509029
4	8	0	-1.090279	-3.501515	-0.659550
5	6	0	3.654005	-0.294931	-1.709084
6	1	0	4.440743	-0.738151	-2.334476
7	1	0	4.103095	-0.093657	-0.728426
8	6	0	3.222380	1.049706	-2.336321
9	1	0	2.775618	0.902658	-3.322369
10	1	0	4.106690	1.686971	-2.457796
11	7	0	2.260734	1.774484	-1.514405
12	1	0	2.603859	2.262493	-0.684194
13	6	0	0.921977	1.695696	-1.687343
14	6	0	0.058916	2.525571	-0.763363
15	6	0	-1.040216	3.147531	-1.375850
16	1	0	-1.189753	2.992033	-2.439610
17	6	0	0.238567	2.673762	0.630791
18	6	0	1.374923	2.042179	1.405762
19	7	0	0.996064	1.157654	2.345709
20	1	0	0.024834	0.836005	2.361001
21	6	0	1.942271	0.413224	3.167551
22	1	0	1.371987	0.000733	4.005331
23	1	0	2.682388	1.109025	3.578484
24	6	0	2.696643	-0.699846	2.411375

25	1	0	3.355018	-0.215967	1.684223
26	1	0	3.345884	-1.212095	3.147892
27	7	0	1.845876	-1.636780	1.682578
28	6	0	1.311059	-2.784786	2.407553
29	1	0	1.301287	-3.643125	1.724487
30	1	0	1.954609	-3.066348	3.262163
31	6	0	-0.120801	-2.594074	2.950078
32	1	0	-0.175402	-1.763236	3.655208
33	1	0	-0.413489	-3.506957	3.486118
34	7	0	-1.092194	-2.335283	1.897567
35	1	0	-1.211221	-3.037889	1.166265
36	6	0	-1.666769	-1.130827	1.709103
37	6	0	-2.554513	-0.944199	0.497935
38	6	0	-3.172139	-1.091101	-1.848378
39	1	0	-2.964889	-1.459649	-2.849471
40	6	0	-2.299692	-1.432753	-0.803470
41	6	0	-1.161062	-2.362458	-1.150121
42	7	0	-0.274879	-1.895756	-2.057703
43	1	0	-0.334737	-0.922016	-2.360341
44	6	0	0.841194	-2.707649	-2.546051
45	1	0	0.557800	-3.201335	-3.485933
46	1	0	1.030572	-3.487480	-1.804409
47	6	0	2.088125	-1.859517	-2.781559
48	1	0	1.853600	-1.091020	-3.536374
49	1	0	2.865972	-2.507976	-3.205450
50	6	0	-0.677486	3.447301	1.359199
51	1	0	-0.547744	3.541259	2.433759
52	6	0	-1.740095	4.093912	0.729107
53	1	0	-2.426286	4.701648	1.313095
54	6	0	-3.676130	-0.125909	0.703155
55	1	0	-3.837309	0.278080	1.697245
56	6	0	-4.555635	0.176353	-0.334281
57	1	0	-5.427671	0.795718	-0.141604
58	6	0	-1.922988	3.941170	-0.646424
59	1	0	-2.753935	4.429076	-1.149113
60	6	0	-4.301612	-0.306200	-1.619180
61	1	0	-4.972483	-0.069708	-2.440934
62	1	0	2.313674	-1.939860	0.833553
63	7	0	2.594975	-1.289837	-1.529763
64	1	0	1.821026	-0.861310	-1.022103

***mac*-1,2-Ph-CO_2 (gas)**

E(RB3LYP) = -1750.73861999 A.U.

Number of Imaginary frequencies = 0

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	8	0	-2.465075	-3.028665	-0.106414
2	8	0	-3.558696	1.478651	0.803965
3	8	0	1.208075	0.754344	1.120102
4	8	0	1.830926	-3.225874	-0.780533
5	8	0	-1.167500	1.433843	-1.765287
6	8	0	1.040406	1.599802	-2.264644
7	7	0	-1.416894	-0.763969	-3.110562
8	1	0	-1.124744	0.505945	-2.241688
9	6	0	-2.892097	-0.815925	-3.215862
10	1	0	-3.205209	-1.382517	-4.109085
11	1	0	-3.225748	0.219881	-3.353521
12	6	0	-3.626572	-1.451800	-2.022961
13	1	0	-3.474563	-2.532444	-2.020673
14	1	0	-4.698742	-1.270076	-2.179067
15	7	0	-3.246697	-0.982618	-0.698223
16	1	0	-3.566005	-0.071444	-0.372104
17	6	0	-2.727188	-1.861662	0.206639
18	6	0	-2.474926	-1.414833	1.633905
19	6	0	-2.335142	-2.486208	2.533070
20	1	0	-2.431339	-3.488760	2.132090
21	6	0	-2.298898	-0.099950	2.124396
22	6	0	-2.484645	1.186485	1.350117
23	7	0	-1.435068	2.042242	1.431784
24	1	0	-0.512744	1.637669	1.592781
25	6	0	-1.512614	3.438248	1.032858
26	1	0	-0.799159	3.991513	1.655783
27	1	0	-2.515385	3.805142	1.276716
28	6	0	-1.258955	3.729372	-0.458053
29	1	0	-2.079862	3.318391	-1.043131
30	1	0	-1.256538	4.819941	-0.595178
31	7	0	-0.007255	3.198224	-0.999791
32	6	0	1.247244	3.905897	-0.787681
33	1	0	1.846893	3.839605	-1.701218
34	1	0	1.008481	4.963214	-0.618002
35	6	0	2.086253	3.416927	0.411367
36	1	0	1.460562	3.320089	1.302165
37	1	0	2.847056	4.179501	0.625383
38	7	0	2.784779	2.151540	0.229121
39	1	0	3.638912	2.163542	-0.312552
40	6	0	2.326396	0.930622	0.629852
41	6	0	3.365861	-0.165391	0.574111
42	6	0	4.216713	-2.401140	0.228267
43	1	0	4.066904	-3.394491	-0.179350
44	6	0	3.193066	-1.457150	0.025209
45	6	0	2.069620	-2.017510	-0.842473
46	7	0	1.479633	-1.229336	-1.783474
47	1	0	1.618649	-0.221088	-1.828700
48	6	0	0.808018	-1.859508	-2.919560

49	1	0	1.245994	-2.854750	-3.034309
50	1	0	1.062679	-1.270701	-3.811168
51	6	0	-0.714704	-2.035641	-2.835976
52	1	0	-1.000373	-2.409241	-1.851311
53	1	0	-1.007465	-2.800747	-3.575678
54	6	0	0.012611	2.029950	-1.718467
55	6	0	-1.997696	0.083619	3.485998
56	1	0	-1.859313	1.095012	3.856420
57	6	0	-1.893482	-0.990674	4.366876
58	1	0	-1.673703	-0.812121	5.416363
59	6	0	4.550087	0.126564	1.279519
60	1	0	4.660048	1.108433	1.731552
61	6	0	5.556089	-0.820608	1.456115
62	1	0	6.452592	-0.564386	2.014583
63	6	0	-2.063747	-2.287562	3.883790
64	1	0	-1.975486	-3.142243	4.549283
65	6	0	5.383284	-2.098107	0.925991
66	1	0	6.147760	-2.859641	1.055962
67	1	0	-1.072185	-0.406710	-4.004113

***mac*(CH_3)-1,2-Ph (gas)**

E(RB3LYP) = -1601.46423059 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.107312	1.094919	-2.580150
2	8	0	0.780753	3.270800	1.408794
3	8	0	-1.774178	-0.916880	2.378151
4	8	0	0.629536	-3.507417	-0.557646
5	7	0	3.260295	0.064433	-1.138133
6	6	0	3.596695	1.483191	-1.309953
7	1	0	4.514832	1.602705	-1.923785
8	1	0	3.833585	1.880220	-0.315599
9	6	0	2.524122	2.382779	-1.947282
10	1	0	2.283911	2.064876	-2.963708
11	1	0	2.962123	3.386323	-2.018195
12	7	0	1.270174	2.499239	-1.219444
13	1	0	1.232207	3.087254	-0.383407
14	6	0	0.138470	1.874264	-1.608169
15	6	0	-1.145896	2.212611	-0.881931
16	6	0	-2.286971	2.237024	-1.700309
17	1	0	-2.163111	2.010494	-2.754099
18	6	0	-1.298950	2.458141	0.502262
19	6	0	-0.156062	2.453334	1.490738

20	7	0	-0.256372	1.539793	2.473196
21	1	0	-0.941809	0.786185	2.376184
22	6	0	0.815231	1.312653	3.435618
23	1	0	0.398963	0.684681	4.229074
24	1	0	1.112942	2.269760	3.878156
25	6	0	2.051584	0.643954	2.795550
26	1	0	2.498443	1.370607	2.110306
27	1	0	2.788106	0.456079	3.598549
28	7	0	1.746341	-0.564574	2.049192
29	6	0	1.850667	-1.859176	2.698317
30	1	0	2.359645	-2.561053	2.024418
31	1	0	2.464834	-1.795320	3.613518
32	6	0	0.485996	-2.473609	3.083542
33	1	0	-0.048065	-1.832899	3.787993
34	1	0	0.648139	-3.448724	3.561433
35	7	0	-0.367857	-2.654926	1.919566
36	1	0	-0.041035	-3.284453	1.184205
37	6	0	-1.353013	-1.791316	1.598280
38	6	0	-2.012646	-1.950162	0.245501
39	6	0	-2.099957	-2.235939	-2.165215
40	1	0	-1.587299	-2.419881	-3.105317
41	6	0	-1.351040	-2.206258	-0.977768
42	6	0	0.123978	-2.514057	-1.111185
43	7	0	0.818359	-1.690388	-1.923383
44	1	0	0.383783	-0.822038	-2.244372
45	6	0	2.214790	-1.927232	-2.275138
46	1	0	2.264371	-2.455395	-3.238765
47	1	0	2.636675	-2.600737	-1.525770
48	6	0	3.014105	-0.626659	-2.410517
49	1	0	2.457687	0.039549	-3.072831
50	1	0	3.969369	-0.865094	-2.919315
51	6	0	4.331075	-0.595802	-0.387866
52	1	0	4.077975	-1.642902	-0.198503
53	1	0	5.298036	-0.571128	-0.928745
54	1	0	4.469922	-0.102956	0.579729
55	6	0	-2.577690	2.726301	1.013435
56	1	0	-2.690341	2.894588	2.080741
57	6	0	-3.693540	2.785687	0.179720
58	1	0	-4.670546	3.013098	0.598155
59	6	0	-3.397742	-1.724619	0.230531
60	1	0	-3.884293	-1.485031	1.170474
61	6	0	-4.134321	-1.793092	-0.949895
62	1	0	-5.209593	-1.636312	-0.927488
63	6	0	-3.546042	2.538141	-1.185777
64	1	0	-4.407393	2.569877	-1.847842
65	6	0	-3.481597	-2.049390	-2.156626
66	1	0	-4.039821	-2.096500	-3.088066
67	1	0	2.116328	-0.546886	1.107541

***mac*(CH_3)-1,2-Ph-CO_2 (gas)**

E(RB3LYP) = -1790.04213781 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.465088	-2.834987	1.056589
2	8	0	3.406925	0.776658	-1.804376
3	8	0	-1.378555	0.179920	-1.441913
4	8	0	-1.684394	-2.630348	1.958466
5	8	0	1.269110	1.938065	0.856422
6	8	0	-0.897211	2.351811	1.370109
7	7	0	1.724667	0.649642	2.928224
8	1	0	1.383251	1.147659	1.932183
9	6	0	3.217287	0.541934	2.798448
10	1	0	3.646139	0.455720	3.806391
11	1	0	3.533050	1.501415	2.377095
12	6	0	3.777315	-0.613504	1.957086
13	1	0	3.626030	-1.571182	2.457632
14	1	0	4.862053	-0.441537	1.905989
15	7	0	3.240817	-0.751288	0.615255
16	1	0	3.496703	-0.074026	-0.104187
17	6	0	2.652096	-1.924660	0.239721
18	6	0	2.218557	-2.121090	-1.197663
19	6	0	1.962689	-3.464584	-1.521986
20	1	0	2.109506	-4.203171	-0.742219
21	6	0	1.983466	-1.132872	-2.183016
22	6	0	2.269589	0.349223	-2.061510
23	7	0	1.227923	1.147916	-2.388221
24	1	0	0.289169	0.762604	-2.273587
25	6	0	1.356758	2.583061	-2.595898
26	1	0	0.593668	2.869478	-3.330180
27	1	0	2.336197	2.772260	-3.048162
28	6	0	1.239798	3.454795	-1.331101
29	1	0	2.103671	3.266359	-0.695638
30	1	0	1.266314	4.508284	-1.648575
31	7	0	0.044629	3.237437	-0.523282
32	6	0	-1.214847	3.849550	-0.904157
33	1	0	-1.739743	4.166366	0.003165
34	1	0	-0.992116	4.748601	-1.495043
35	6	0	-2.154123	2.962269	-1.746102
36	1	0	-1.610080	2.496861	-2.571399
37	1	0	-2.932775	3.601790	-2.184269
38	7	0	-2.831453	1.899684	-1.015206
39	1	0	-3.584631	2.173655	-0.397686
40	6	0	-2.418591	0.604601	-0.930587
41	6	0	-3.434649	-0.319273	-0.298329

42	6	0	-4.209028	-2.174493	1.044443
43	1	0	-3.996366	-2.920943	1.801349
44	6	0	-3.176722	-1.279803	0.705448
45	6	0	-1.941386	-1.487029	1.574068
46	7	0	-1.261976	-0.406891	2.060816
47	1	0	-1.409293	0.549677	1.725413
48	6	0	-0.501386	-0.561852	3.296616
49	1	0	-0.817445	-1.510743	3.738177
50	1	0	-0.802182	0.238896	3.980087
51	6	0	1.028084	-0.650506	3.195007
52	1	0	1.301685	-1.359965	2.414325
53	1	0	1.412628	-1.035395	4.150661
54	6	0	1.410390	1.687818	3.949441
55	1	0	0.378242	2.016094	3.826243
56	1	0	1.575791	1.291191	4.957398
57	1	0	2.061463	2.548002	3.781430
58	6	0	0.117305	2.472986	0.635226
59	6	0	1.510361	-1.533476	-3.444776
60	1	0	1.326559	-0.771901	-4.196601
61	6	0	1.289195	-2.873668	-3.755592
62	1	0	0.934363	-3.148912	-4.745535
63	6	0	-4.707326	-0.283942	-0.901039
64	1	0	-4.886416	0.432011	-1.698198
65	6	0	-5.719841	-1.169327	-0.538689
66	1	0	-6.687821	-1.119627	-1.030505
67	6	0	1.517969	-3.847275	-2.784202
68	1	0	1.341490	-4.897627	-3.000405
69	6	0	-5.464047	-2.125743	0.442619
70	1	0	-6.232522	-2.835180	0.738316

***mac*-1,2-Ph (DMSO)**

E(RB3LYP) = -1562.18082128 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.435022	0.868993	-2.600729
2	8	0	2.993706	2.033002	1.086869
3	8	0	-1.499494	0.231944	2.474907
4	8	0	-1.749955	-3.352280	-0.498475
5	6	0	3.534056	-0.954909	-1.839887
6	1	0	4.197707	-1.517833	-2.508525
7	1	0	4.085361	-0.792972	-0.905633
8	6	0	3.245227	0.416153	-2.487925
9	1	0	2.712411	0.302900	-3.434122

10	1	0	4.196847	0.918196	-2.694882
11	7	0	2.455251	1.299717	-1.632643
12	1	0	2.931495	1.778212	-0.868644
13	6	0	1.121350	1.467186	-1.747379
14	6	0	0.469476	2.486061	-0.839251
15	6	0	-0.514239	3.285940	-1.443417
16	1	0	-0.733110	3.131245	-2.495076
17	6	0	0.735420	2.658155	0.537775
18	6	0	1.774624	1.864690	1.299343
19	7	0	1.286292	1.030481	2.229307
20	1	0	0.276085	0.876665	2.267060
21	6	0	2.115156	0.171111	3.070076
22	1	0	1.514737	-0.087841	3.946559
23	1	0	2.979441	0.744331	3.420759
24	6	0	2.623975	-1.096370	2.358872
25	1	0	3.321211	-0.787471	1.573993
26	1	0	3.204303	-1.674919	3.101314
27	7	0	1.579477	-1.899829	1.724022
28	6	0	0.856293	-2.858191	2.559851
29	1	0	0.677667	-3.761931	1.965179
30	1	0	1.451769	-3.168929	3.436253
31	6	0	-0.502644	-2.353608	3.084963
32	1	0	-0.384608	-1.474851	3.719607
33	1	0	-0.955450	-3.146482	3.693216
34	7	0	-1.430172	-1.999395	2.015375
35	1	0	-1.702196	-2.728665	1.357096
36	6	0	-1.813151	-0.737317	1.750277
37	6	0	-2.698847	-0.493706	0.549622
38	6	0	-3.392430	-0.706334	-1.771903
39	1	0	-3.269661	-1.168681	-2.747654
40	6	0	-2.556935	-1.104842	-0.716618
41	6	0	-1.589171	-2.226240	-1.011038
42	7	0	-0.606279	-1.947544	-1.884648
43	1	0	-0.504469	-0.990980	-2.227300
44	6	0	0.347012	-2.956105	-2.358424
45	1	0	-0.066225	-3.468254	-3.236843
46	1	0	0.475882	-3.698136	-1.566137
47	6	0	1.681723	-2.317175	-2.725846
48	1	0	1.503888	-1.551633	-3.498446
49	1	0	2.317599	-3.088631	-3.176656
50	6	0	0.017513	3.623512	1.260837
51	1	0	0.212866	3.740681	2.323359
52	6	0	-0.932897	4.433285	0.637962
53	1	0	-1.465533	5.184300	1.214712
54	6	0	-3.680050	0.497742	0.712824
55	1	0	-3.765530	0.985556	1.678309
56	6	0	-4.528800	0.861058	-0.331742
57	1	0	-5.292257	1.617002	-0.170646
58	6	0	-1.199639	4.262795	-0.722496
59	1	0	-1.942201	4.880791	-1.219503

60	6	0	-4.381944	0.259428	-1.583564
61	1	0	-5.027451	0.541078	-2.410748
62	1	0	1.970455	-2.372290	0.914734
63	7	0	2.365623	-1.786734	-1.541038
64	1	0	1.706915	-1.244519	-0.982014

mac-1,2-Ph-CO_2 (DMSO)

E(RB3LYP) = -1750.76767117 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	4.094552	-2.753829	-0.169063
2	8	0	3.771873	1.167120	-1.641567
3	8	0	-1.047610	0.572729	-0.702772
4	8	0	-3.524053	-1.915423	2.518038
5	8	0	1.418526	1.381959	1.569227
6	8	0	-0.670382	1.850377	2.271487
7	7	0	1.412679	-0.541302	3.245168
8	1	0	1.229596	0.281847	2.530341
9	6	0	2.909982	-0.672306	3.277213
10	1	0	3.199810	-1.196749	4.191248
11	1	0	3.280858	0.353608	3.333964
12	6	0	3.518956	-1.415065	2.089675
13	1	0	3.374034	-2.494188	2.202038
14	1	0	4.602055	-1.246427	2.131683
15	7	0	2.983458	-1.032129	0.781982
16	1	0	2.390328	-0.205958	0.697853
17	6	0	3.279115	-1.823698	-0.280790
18	6	0	2.499199	-1.676944	-1.566073
19	6	0	2.116652	-2.900320	-2.143606
20	1	0	2.420220	-3.819727	-1.654312
21	6	0	2.108726	-0.477940	-2.195476
22	6	0	2.565700	0.895644	-1.762760
23	7	0	1.562535	1.790891	-1.634712
24	1	0	0.621338	1.420853	-1.497823
25	6	0	1.754815	3.214832	-1.398907
26	1	0	1.049957	3.756314	-2.040880
27	1	0	2.764719	3.480405	-1.723118
28	6	0	1.573238	3.631656	0.071257
29	1	0	2.400773	3.236012	0.660106
30	1	0	1.616342	4.728881	0.116301
31	7	0	0.333709	3.186082	0.701928
32	6	0	-0.901616	3.917259	0.462166
33	1	0	-1.495904	3.926174	1.379552

34	1	0	-0.637995	4.954467	0.221486
35	6	0	-1.771333	3.395401	-0.703015
36	1	0	-1.148459	3.172067	-1.573836
37	1	0	-2.462402	4.192606	-0.994173
38	7	0	-2.609869	2.221314	-0.432442
39	1	0	-3.593974	2.392366	-0.267772
40	6	0	-2.228795	0.934490	-0.547327
41	6	0	-3.353501	-0.072856	-0.616008
42	6	0	-4.594435	-2.060947	-0.013491
43	1	0	-4.766699	-2.873928	0.683028
44	6	0	-3.556273	-1.154836	0.270299
45	6	0	-2.857837	-1.426476	1.589128
46	7	0	-1.526726	-1.207753	1.721918
47	1	0	-1.036013	-0.663795	1.015567
48	6	0	-0.899071	-1.495400	3.013209
49	1	0	-1.390839	-2.387715	3.403823
50	1	0	-1.107250	-0.684776	3.724065
51	6	0	0.608898	-1.769091	2.947930
52	1	0	0.903335	-2.137486	1.964011
53	1	0	0.875554	-2.522961	3.693088
54	6	0	0.334166	2.093111	1.560129
55	6	0	1.345279	-0.540955	-3.374014
56	1	0	1.064255	0.384748	-3.867366
57	6	0	0.969157	-1.762014	-3.933245
58	1	0	0.383629	-1.781931	-4.848232
59	6	0	-4.195690	0.067144	-1.734295
60	1	0	-4.041016	0.906099	-2.407129
61	6	0	-5.203845	-0.855654	-2.009304
62	1	0	-5.828522	-0.729949	-2.889126
63	6	0	1.357226	-2.950236	-3.311642
64	1	0	1.072505	-3.911259	-3.730935
65	6	0	-5.397947	-1.933532	-1.144188
66	1	0	-6.177070	-2.665078	-1.339137
67	1	0	1.118492	-0.175310	4.154770

***mac*(CH_3)-1,2-Ph (DMSO)**

E(RB3LYP) = -1601.48444618 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.150713	0.565894	-2.592320
2	8	0	0.578497	3.634604	0.855623
3	8	0	-1.713013	-0.576172	2.411565
4	8	0	0.777092	-3.703865	-0.029534

5	7	0	3.282029	0.075833	-1.209601
6	6	0	3.442152	1.447066	-1.715067
7	1	0	4.295321	1.513106	-2.419918
8	1	0	3.698363	2.079393	-0.857468
9	6	0	2.236335	2.067393	-2.434991
10	1	0	1.951585	1.491375	-3.316550
11	1	0	2.555421	3.056246	-2.784496
12	7	0	1.031220	2.256812	-1.631824
13	1	0	1.005746	3.035231	-0.974157
14	6	0	-0.097997	1.544106	-1.818079
15	6	0	-1.358935	2.011514	-1.124360
16	6	0	-2.536829	1.869746	-1.877410
17	1	0	-2.464903	1.442480	-2.872129
18	6	0	-1.452200	2.537317	0.183713
19	6	0	-0.261833	2.741253	1.091790
20	7	0	-0.219047	1.936544	2.164433
21	1	0	-0.854496	1.135841	2.193185
22	6	0	0.896209	1.913338	3.107335
23	1	0	0.539598	1.407280	4.008895
24	1	0	1.157697	2.940588	3.381096
25	6	0	2.138517	1.203801	2.534095
26	1	0	2.525923	1.815785	1.714021
27	1	0	2.911728	1.188637	3.322857
28	7	0	1.858793	-0.127056	2.010840
29	6	0	1.994644	-1.270820	2.903599
30	1	0	2.532809	-2.071620	2.381041
31	1	0	2.592762	-1.015551	3.794082
32	6	0	0.644542	-1.836711	3.392115
33	1	0	0.086464	-1.086967	3.954760
34	1	0	0.828470	-2.693077	4.052210
35	7	0	-0.194088	-2.274292	2.282016
36	1	0	0.145823	-3.048753	1.712946
37	6	0	-1.240950	-1.567782	1.815913
38	6	0	-1.899214	-2.040211	0.539910
39	6	0	-1.957496	-2.828396	-1.759061
40	1	0	-1.430699	-3.173860	-2.644577
41	6	0	-1.220513	-2.508647	-0.607677
42	6	0	0.268684	-2.763450	-0.676647
43	7	0	0.966614	-1.976541	-1.509226
44	1	0	0.495470	-1.183783	-1.951945
45	6	0	2.383200	-2.194469	-1.808024
46	1	0	2.473154	-2.949185	-2.601259
47	1	0	2.860581	-2.610195	-0.917470
48	6	0	3.072527	-0.911487	-2.279585
49	1	0	2.459301	-0.465451	-3.065979
50	1	0	4.033014	-1.192378	-2.749499
51	6	0	4.462298	-0.277804	-0.411347
52	1	0	4.361863	-1.287889	-0.004790
53	1	0	5.392905	-0.243167	-1.009129
54	1	0	4.570130	0.416824	0.427704

55	6	0	-2.707006	2.908142	0.690603
56	1	0	-2.772663	3.295450	1.703746
57	6	0	-3.862053	2.791702	-0.083623
58	1	0	-4.820959	3.099009	0.324397
59	6	0	-3.296429	-1.908350	0.491133
60	1	0	-3.808432	-1.518980	1.365167
61	6	0	-4.021867	-2.260744	-0.645809
62	1	0	-5.104229	-2.166638	-0.648476
63	6	0	-3.774837	2.267906	-1.375277
64	1	0	-4.665702	2.163197	-1.988258
65	6	0	-3.348507	-2.720307	-1.780047
66	1	0	-3.898471	-2.987037	-2.678291
67	1	0	2.318217	-0.273347	1.119944

***mac*(CH_3)-1,2-Ph-(CO_2) (DMSO)**

E(RB3LYP) = -1790.08213286 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.108011	-0.141310	-2.533195
2	8	0	-3.551322	-2.047105	1.100962
3	8	0	1.261810	-1.256612	0.391202
4	8	0	1.597827	1.261259	-2.930054
5	8	0	-1.134058	1.182763	1.563500
6	8	0	1.003212	1.749521	2.024173
7	7	0	-1.506258	3.218920	0.054837
8	1	0	-1.162757	2.377631	0.660884
9	6	0	-3.003367	3.018220	0.005222
10	1	0	-3.461599	3.965183	-0.293740
11	1	0	-3.292457	2.806905	1.037230
12	6	0	-3.523107	1.936494	-0.934721
13	1	0	-3.432209	2.254494	-1.978373
14	1	0	-4.599102	1.854710	-0.737437
15	7	0	-2.883652	0.628011	-0.797354
16	1	0	-2.192820	0.474909	-0.062474
17	6	0	-3.214124	-0.336118	-1.692674
18	6	0	-2.402061	-1.606702	-1.758330
19	6	0	-2.065774	-2.011697	-3.061483
20	1	0	-2.409766	-1.409351	-3.895902
21	6	0	-1.959889	-2.382508	-0.668732
22	6	0	-2.357138	-2.121121	0.764905
23	7	0	-1.316935	-2.074837	1.624371
24	1	0	-0.384885	-1.921326	1.232701
25	6	0	-1.457457	-1.985958	3.070559

26	1	0	-0.725883	-2.666964	3.520781
27	1	0	-2.453457	-2.347632	3.340200
28	6	0	-1.277738	-0.561982	3.624972
29	1	0	-2.106128	0.061585	3.289923
30	1	0	-1.314672	-0.620494	4.721437
31	7	0	-0.037336	0.106060	3.235448
32	6	0	1.203314	-0.243551	3.915753
33	1	0	1.793242	0.663050	4.078251
34	1	0	0.944000	-0.654789	4.898308
35	6	0	2.071440	-1.291571	3.190551
36	1	0	1.466201	-2.143303	2.872135
37	1	0	2.821397	-1.666929	3.895974
38	7	0	2.800395	-0.797053	2.026031
39	1	0	3.672231	-0.316624	2.208240
40	6	0	2.377519	-0.837648	0.742854
41	6	0	3.421663	-0.443167	-0.272311
42	6	0	4.219123	0.554049	-2.328648
43	1	0	4.036959	1.190604	-3.187576
44	6	0	3.182912	0.386239	-1.390814
45	6	0	1.956491	1.214587	-1.742339
46	7	0	1.411476	2.035245	-0.807439
47	1	0	1.564333	1.904816	0.198812
48	6	0	0.703960	3.244362	-1.227159
49	1	0	1.029592	3.468307	-2.245988
50	1	0	1.047235	4.065542	-0.592599
51	6	0	-0.828153	3.194435	-1.285215
52	1	0	-1.138146	2.283506	-1.796974
53	1	0	-1.191168	4.058242	-1.852373
54	6	0	-1.212573	4.457376	0.838903
55	1	0	-0.160946	4.471569	1.119816
56	1	0	-1.462164	5.336900	0.240782
57	1	0	-1.817960	4.441530	1.746346
58	6	0	-0.035769	1.059819	2.228648
59	6	0	-1.196440	-3.536106	-0.915182
60	1	0	-0.874532	-4.143048	-0.074021
61	6	0	-0.867242	-3.925133	-2.213411
62	1	0	-0.279881	-4.824418	-2.377185
63	6	0	4.676401	-1.068014	-0.139505
64	1	0	4.843527	-1.739271	0.697647
65	6	0	5.692960	-0.882060	-1.074848
66	1	0	6.647746	-1.383777	-0.945681
67	6	0	-1.302340	-3.154752	-3.293745
68	1	0	-1.051943	-3.440552	-4.311627
69	6	0	5.460782	-0.061279	-2.178153
70	1	0	6.236153	0.099149	-2.922068

***mac*-Fu (gas)**

E(RB3LYP) = -1557.71147648 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.441093	-1.621913	-1.032030
2	8	0	1.964367	-4.136071	-1.686595
3	8	0	4.559094	2.059510	-0.862412
4	8	0	-2.047890	3.941950	-1.622170
5	6	0	-3.553396	0.057149	2.713467
6	1	0	-4.355235	0.467037	3.340659
7	1	0	-2.877557	-0.483747	3.392030
8	6	0	-4.179715	-0.941715	1.722495
9	1	0	-4.899167	-0.456534	1.059163
10	1	0	-4.725630	-1.715853	2.282947
11	7	0	-3.161956	-1.544900	0.871125
12	1	0	-2.326306	-1.918355	1.304648
13	6	0	-3.386960	-1.854821	-0.443155
14	6	0	-2.255411	-2.494707	-1.149134
15	6	0	-2.189981	-3.094280	-2.378181
16	1	0	-3.012253	-3.178161	-3.074319
17	6	0	-0.854671	-3.566922	-2.529958
18	1	0	-0.422075	-4.090890	-3.370168
19	6	0	-0.183681	-3.220229	-1.387764
20	6	0	1.234130	-3.412740	-1.008783
21	7	0	1.649452	-2.756540	0.113627
22	1	0	1.052559	-2.048851	0.524366
23	6	0	3.038862	-2.783025	0.545602
24	1	0	3.631577	-2.057068	-0.026749
25	1	0	3.440208	-3.774569	0.317733
26	6	0	3.142234	-2.511625	2.048356
27	1	0	2.561417	-3.279036	2.574102
28	1	0	4.193942	-2.635021	2.354195
29	7	0	2.629292	-1.185244	2.446584
30	6	0	3.654364	-0.157650	2.693726
31	1	0	3.196697	0.623764	3.312808
32	1	0	4.509951	-0.564610	3.260365
33	6	0	4.201310	0.483866	1.419374
34	1	0	4.689231	-0.261483	0.778058
35	1	0	4.974178	1.213506	1.685344
36	7	0	3.143280	1.167654	0.690144
37	1	0	2.185702	0.915587	0.900593
38	6	0	3.418640	1.904714	-0.423690
39	6	0	2.262933	2.543500	-1.091577
40	6	0	2.165537	3.154443	-2.313181
41	1	0	2.976642	3.268283	-3.018099
42	6	0	0.815050	3.588025	-2.445930
43	1	0	0.358944	4.111817	-3.273745
44	6	0	0.171683	3.224484	-1.293408

45	6	0	-1.218857	3.469027	-0.846115
46	7	0	-1.483181	3.146618	0.455577
47	1	0	-0.709172	2.860827	1.040589
48	6	0	-2.773050	3.397987	1.091380
49	1	0	-3.330460	4.074824	0.438885
50	1	0	-2.590339	3.895956	2.050355
51	6	0	-3.576347	2.114816	1.328876
52	1	0	-3.893942	1.699242	0.359163
53	1	0	-4.484015	2.379217	1.886993
54	8	0	-1.030587	-2.562962	-0.529080
55	8	0	1.046357	2.576858	-0.453834
56	1	0	2.070331	-1.284540	3.288481
57	7	0	-2.800584	1.169945	2.140224
58	1	0	-2.047377	0.795168	1.565191

***mac*-Fu-CO_2 (gas)**

E(RB3LYP) = -1746.31945632 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-5.188704	1.168306	-0.772793
2	8	0	-1.061196	-4.374496	-1.571036
3	8	0	4.840670	-1.696657	-0.904827
4	8	0	1.033611	3.971363	-2.180349
5	8	0	-0.585459	-0.295337	1.526005
6	8	0	1.298062	0.818938	2.053218
7	7	0	-1.351891	2.224966	1.804258
8	1	0	-1.023333	1.243916	1.464071
9	6	0	-2.642855	2.030722	2.549562
10	1	0	-2.842036	2.932956	3.136312
11	1	0	-2.466507	1.198357	3.237564
12	6	0	-3.831445	1.741657	1.633255
13	1	0	-4.099754	2.613655	1.028802
14	1	0	-4.698340	1.536354	2.278720
15	7	0	-3.550286	0.636180	0.741665
16	1	0	-2.852515	-0.052823	1.005728
17	6	0	-4.270060	0.434113	-0.413166
18	6	0	-3.820430	-0.738359	-1.187225
19	6	0	-4.254093	-1.392770	-2.311816
20	1	0	-5.107122	-1.115093	-2.914910
21	6	0	-3.364591	-2.495222	-2.507447
22	1	0	-3.392471	-3.237998	-3.291935
23	6	0	-2.441562	-2.439109	-1.495023
24	6	0	-1.272083	-3.263851	-1.082334

25	7	0	-0.523734	-2.669064	-0.118189
26	1	0	-0.789032	-1.746616	0.224705
27	6	0	0.510350	-3.343204	0.649639
28	1	0	1.487914	-3.258698	0.156875
29	1	0	0.262030	-4.409897	0.698772
30	6	0	0.573150	-2.758500	2.074037
31	1	0	-0.446096	-2.667959	2.466532
32	1	0	1.105973	-3.473902	2.708475
33	7	0	1.263278	-1.469745	2.219221
34	6	0	2.614453	-1.476216	2.789607
35	1	0	2.765870	-0.518978	3.295046
36	1	0	2.668019	-2.265594	3.548769
37	6	0	3.743879	-1.696090	1.771231
38	1	0	3.653706	-2.661833	1.260417
39	1	0	4.705730	-1.703704	2.304088
40	7	0	3.699365	-0.631887	0.784079
41	1	0	3.087001	0.149791	1.003622
42	6	0	4.147717	-0.765670	-0.493937
43	6	0	3.688719	0.326865	-1.389444
44	6	0	3.921200	0.671834	-2.695929
45	1	0	4.592587	0.160881	-3.371293
46	6	0	3.101164	1.810108	-2.968092
47	1	0	3.012582	2.357574	-3.895784
48	6	0	2.418260	2.083100	-1.810155
49	6	0	1.404430	3.079258	-1.416940
50	7	0	0.921313	2.914286	-0.140930
51	1	0	1.276891	2.162864	0.453612
52	6	0	-0.000827	3.860126	0.439456
53	1	0	-0.125170	4.677744	-0.276768
54	1	0	0.425398	4.285583	1.361181
55	6	0	-1.386200	3.283093	0.735257
56	1	0	-1.828404	2.835845	-0.156998
57	1	0	-2.039561	4.087435	1.091203
58	6	0	0.645125	-0.260665	1.926006
59	8	0	-2.718519	-1.372980	-0.690407
60	8	0	2.777301	1.186085	-0.848191
61	1	0	-0.611619	2.447886	2.480250

***mac*(CH_3)-Fu (gas)**

E(RB3LYP) = -1597.02227961 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.003515	-3.965669	-2.434573

2	8	0	5.012110	-1.751097	0.051961
3	8	0	1.624494	4.055345	-2.119696
4	8	0	-4.692050	1.787846	-0.446607
5	7	0	-2.970817	-1.795528	1.762937
6	6	0	-3.103941	-3.011348	0.940913
7	1	0	-4.135002	-3.409304	0.982178
8	1	0	-2.447919	-3.784622	1.355420
9	6	0	-2.708142	-2.781685	-0.518482
10	1	0	-3.261218	-1.935344	-0.946618
11	1	0	-2.949115	-3.662553	-1.118567
12	7	0	-1.273247	-2.562221	-0.646750
13	1	0	-0.823722	-1.950915	0.023252
14	6	0	-0.526662	-3.213143	-1.582588
15	6	0	0.938689	-3.008094	-1.536484
16	6	0	1.911648	-3.567719	-2.320923
17	1	0	1.729758	-4.237221	-3.149105
18	6	0	3.157992	-3.104710	-1.816405
19	1	0	4.152430	-3.334899	-2.170701
20	6	0	2.871783	-2.287361	-0.755587
21	6	0	3.797181	-1.561907	0.139642
22	7	0	3.251085	-0.708784	1.053133
23	1	0	2.275373	-0.447694	0.985154
24	6	0	4.116621	0.074102	1.923946
25	1	0	4.745119	0.748674	1.326759
26	1	0	4.804354	-0.605939	2.437617
27	6	0	3.315192	0.854779	2.961330
28	1	0	2.741268	0.152427	3.578057
29	1	0	4.039308	1.360219	3.624577
30	7	0	2.360439	1.804218	2.368639
31	6	0	2.960660	2.988884	1.719209
32	1	0	2.414542	3.882337	2.044353
33	1	0	4.009712	3.120688	2.026254
34	6	0	2.889123	2.912514	0.189521
35	1	0	3.492282	2.075480	-0.186920
36	1	0	3.282140	3.828652	-0.260332
37	7	0	1.504636	2.766950	-0.226269
38	1	0	0.919982	2.169078	0.344381
39	6	0	0.979415	3.362055	-1.332818
40	6	0	-0.471376	3.142257	-1.537506
41	6	0	-1.312071	3.546068	-2.539689
42	1	0	-1.014235	4.110266	-3.411808
43	6	0	-2.614529	3.084936	-2.190241
44	1	0	-3.538453	3.216775	-2.734971
45	6	0	-2.490068	2.428590	-0.994887
46	6	0	-3.500786	1.780996	-0.132173
47	7	0	-3.028037	1.216562	1.018028
48	1	0	-2.028482	1.153909	1.150694
49	6	0	-3.908590	0.539267	1.958825
50	1	0	-4.869015	1.062080	1.942457
51	1	0	-3.483284	0.654109	2.961186

52	6	0	-4.155261	-0.935862	1.620354
53	1	0	-4.503273	-0.978692	0.584842
54	1	0	-4.985547	-1.309680	2.252102
55	6	0	-2.720020	-2.128745	3.166014
56	1	0	-2.593373	-1.216523	3.757577
57	1	0	-3.543925	-2.714081	3.618470
58	1	0	-1.796660	-2.710672	3.249979
59	8	0	1.510928	-2.212329	-0.571985
60	8	0	-1.179713	2.451689	-0.584437
61	1	0	1.719356	2.105541	3.096549

***mac*(CH_3)-Fu-CO_2 (gas)**

E(RB3LYP) = -1785.62670262 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.951382	0.223212	1.409200
2	8	0	0.284509	4.743382	0.703268
3	8	0	4.856072	0.977928	1.103293
4	8	0	-0.097097	-3.628245	2.698251
5	8	0	-0.487847	0.140399	-1.750313
6	8	0	1.228777	-1.320169	-1.750761
7	7	0	-1.945185	-2.150808	-1.679989
8	1	0	-1.305227	-1.302458	-1.496990
9	6	0	-3.282476	-1.585909	-2.108738
10	1	0	-3.839754	-2.397314	-2.588198
11	1	0	-3.048573	-0.831463	-2.865820
12	6	0	-4.134762	-0.980273	-0.997409
13	1	0	-4.480967	-1.735803	-0.285979
14	1	0	-5.040568	-0.580887	-1.478468
15	7	0	-3.416209	0.054335	-0.284688
16	1	0	-2.606627	0.486142	-0.719745
17	6	0	-3.926047	0.621480	0.859954
18	6	0	-3.125314	1.754672	1.358834
19	6	0	-3.226524	2.642156	2.399345
20	1	0	-3.996986	2.640861	3.157513
21	6	0	-2.129980	3.550313	2.265521
22	1	0	-1.883877	4.389953	2.899800
23	6	0	-1.428628	3.156850	1.154977
24	6	0	-0.234448	3.661759	0.426114
25	7	0	0.173004	2.830076	-0.567347
26	1	0	-0.311213	1.947336	-0.715881
27	6	0	1.194577	3.173544	-1.542145
28	1	0	2.189411	3.167283	-1.080002

29	1	0	1.016024	4.193484	-1.906955
30	6	0	1.127408	2.188806	-2.720137
31	1	0	0.095660	2.133170	-3.082494
32	1	0	1.742021	2.589344	-3.533852
33	7	0	1.599691	0.830220	-2.438290
34	6	0	2.988256	0.500425	-2.781437
35	1	0	3.016396	-0.547862	-3.091662
36	1	0	3.281059	1.110367	-3.643971
37	6	0	4.018013	0.718135	-1.659839
38	1	0	4.054237	1.763174	-1.331405
39	1	0	5.016700	0.469541	-2.047804
40	7	0	3.670702	-0.126639	-0.531134
41	1	0	2.925847	-0.799824	-0.701865
42	6	0	4.024429	0.139145	0.755362
43	6	0	3.274089	-0.682355	1.741214
44	6	0	3.304676	-0.838853	3.103417
45	1	0	3.993777	-0.350362	3.777576
46	6	0	2.254067	-1.751033	3.431502
47	1	0	1.969830	-2.111388	4.410079
48	6	0	1.648580	-2.088593	2.247405
49	6	0	0.509843	-2.946876	1.869876
50	7	0	0.201119	-2.914027	0.531871
51	1	0	0.731470	-2.322614	-0.115247
52	6	0	-0.819772	-3.774544	-0.015590
53	1	0	-1.129681	-4.455750	0.783300
54	1	0	-0.406957	-4.386439	-0.826443
55	6	0	-2.085435	-3.039332	-0.463896
56	1	0	-2.438329	-2.405349	0.350628
57	1	0	-2.862829	-3.772611	-0.710952
58	6	0	-1.319817	-2.854899	-2.845446
59	1	0	-0.261424	-3.005304	-2.638936
60	1	0	-1.839940	-3.800843	-3.018775
61	1	0	-1.412261	-2.210135	-3.721027
62	6	0	0.749573	-0.165013	-1.959632
63	8	0	-2.031475	2.065267	0.603137
64	8	0	2.269579	-1.443521	1.220814

***mac*-Fu (DMSO)**

E(RB3LYP) = -1557.75046893 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.799864	-2.248846	-1.330439
2	8	0	3.031274	-3.291656	-1.623853
3	8	0	3.857006	2.788402	-1.116821

4	8	0	-3.047212	3.115590	-1.413222
5	6	0	-3.525981	-0.979425	2.671220
6	1	0	-4.429830	-0.848742	3.278666
7	1	0	-2.773999	-1.445734	3.321033
8	6	0	-3.867685	-1.948147	1.523373
9	1	0	-4.649301	-1.545741	0.876223
10	1	0	-4.244228	-2.888205	1.950243
11	7	0	-2.701781	-2.209011	0.684328
12	1	0	-1.818691	-2.406126	1.141996
13	6	0	-2.757839	-2.340707	-0.663278
14	6	0	-1.469270	-2.608182	-1.339257
15	6	0	-1.186552	-2.978317	-2.628140
16	1	0	-1.909295	-3.124315	-3.418058
17	6	0	0.227059	-3.137728	-2.703449
18	1	0	0.812999	-3.422408	-3.565582
19	6	0	0.719612	-2.847457	-1.457719
20	6	0	2.106596	-2.817449	-0.943115
21	7	0	2.283983	-2.265273	0.277033
22	1	0	1.518919	-1.764696	0.716266
23	6	0	3.597973	-2.141547	0.897526
24	1	0	4.209406	-1.421773	0.340161
25	1	0	4.108277	-3.108523	0.839234
26	6	0	3.456955	-1.732118	2.366584
27	1	0	2.889224	-2.511219	2.887848
28	1	0	4.464701	-1.711244	2.811663
29	7	0	2.753050	-0.454037	2.560072
30	6	0	3.603455	0.740491	2.673148
31	1	0	3.055341	1.481920	3.265537
32	1	0	4.542942	0.524829	3.208156
33	6	0	3.967788	1.369136	1.326286
34	1	0	4.566960	0.684271	0.714775
35	1	0	4.582622	2.259128	1.500745
36	7	0	2.761916	1.758108	0.603633
37	1	0	1.881537	1.374696	0.929359
38	6	0	2.801977	2.434598	-0.564620
39	6	0	1.496614	2.761258	-1.181060
40	6	0	1.179389	3.224631	-2.431417
41	1	0	1.881896	3.445540	-3.222223
42	6	0	-0.239765	3.343089	-2.472561
43	1	0	-0.849276	3.680995	-3.298370
44	6	0	-0.699545	2.953357	-1.241780
45	6	0	-2.067591	2.912300	-0.679901
46	7	0	-2.152709	2.658794	0.649055
47	1	0	-1.290435	2.560698	1.170833
48	6	0	-3.417446	2.602972	1.381269
49	1	0	-4.143743	3.217563	0.843837
50	1	0	-3.247139	3.043534	2.368285
51	6	0	-3.959562	1.178225	1.535494
52	1	0	-4.195502	0.775826	0.536733
53	1	0	-4.901144	1.232667	2.096289

54	8	0	-0.309557	-2.523163	-0.613428
55	8	0	0.354369	2.591350	-0.443584
56	1	0	2.177750	-0.519663	3.393789
57	7	0	-3.024257	0.342870	2.294008
58	1	0	-2.166597	0.229261	1.754814

***mac*-Fu-CO_2 (DMSO)**

E(RB3LYP) = -1746.36585789 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	4.971711	1.008742	1.218786
2	8	0	0.675481	-4.454843	1.535026
3	8	0	-4.795509	-1.371136	1.244731
4	8	0	-0.787969	4.288131	1.746211
5	8	0	0.562724	-0.406448	-1.672366
6	8	0	-1.380571	0.704745	-1.940003
7	7	0	1.625161	2.130921	-2.057055
8	1	0	1.152292	1.240442	-1.716772
9	6	0	3.015025	1.782954	-2.541023
10	1	0	3.364112	2.609929	-3.162560
11	1	0	2.898931	0.898580	-3.172630
12	6	0	4.018922	1.537266	-1.419237
13	1	0	4.205500	2.444263	-0.838719
14	1	0	4.969211	1.265239	-1.897310
15	7	0	3.565137	0.489718	-0.519729
16	1	0	2.894056	-0.189734	-0.863248
17	6	0	4.088361	0.297686	0.721877
18	6	0	3.499068	-0.845788	1.448975
19	6	0	3.723332	-1.446390	2.661684
20	1	0	4.452188	-1.144249	3.400451
21	6	0	2.810797	-2.543824	2.744342
22	1	0	2.701854	-3.243515	3.560874
23	6	0	2.087370	-2.538805	1.578819
24	6	0	1.011855	-3.383331	1.003027
25	7	0	0.482670	-2.884554	-0.132082
26	1	0	0.790248	-1.972999	-0.477607
27	6	0	-0.459995	-3.593377	-0.987726
28	1	0	-1.429095	-3.705068	-0.486536
29	1	0	-0.078399	-4.601927	-1.191665
30	6	0	-0.612509	-2.835251	-2.315033
31	1	0	0.380202	-2.649535	-2.737481
32	1	0	-1.148598	-3.485402	-3.012256
33	7	0	-1.342346	-1.565667	-2.236765

34	6	0	-2.759088	-1.562996	-2.622659
35	1	0	-2.970794	-0.629527	-3.151401
36	1	0	-2.925697	-2.384951	-3.325171
37	6	0	-3.750963	-1.717511	-1.458448
38	1	0	-3.588734	-2.656221	-0.916482
39	1	0	-4.772086	-1.743037	-1.862492
40	7	0	-3.582114	-0.592677	-0.549180
41	1	0	-2.922333	0.122060	-0.863875
42	6	0	-4.033563	-0.541024	0.720917
43	6	0	-3.512270	0.624198	1.478336
44	6	0	-3.695520	1.132851	2.739490
45	1	0	-4.357301	0.739262	3.498051
46	6	0	-2.839944	2.273148	2.844870
47	1	0	-2.718077	2.923194	3.699743
48	6	0	-2.189135	2.383322	1.641195
49	6	0	-1.179275	3.310825	1.089273
50	7	0	-0.746181	3.001580	-0.162587
51	1	0	-1.104235	2.170612	-0.647090
52	6	0	0.173677	3.853589	-0.892406
53	1	0	0.282207	4.785159	-0.332543
54	1	0	-0.258780	4.102879	-1.869388
55	6	0	1.575053	3.267345	-1.068840
56	1	0	1.963466	2.897056	-0.119624
57	1	0	2.240480	4.045646	-1.451982
58	6	0	-0.693774	-0.365448	-1.942488
59	8	0	2.505545	-1.508095	0.790345
60	8	0	-2.599135	1.385826	0.811635
61	1	0	1.080342	2.394590	-2.885083

***mac*(CH_3)-Fu (DMSO)**

E(RB3LYP) = -1597.05858993 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.890696	-3.483852	-2.469368
2	8	0	4.512845	-2.374651	-0.184533
3	8	0	2.606867	3.423324	-2.021438
4	8	0	-4.138908	2.467931	-0.802226
5	7	0	-3.189171	-1.111778	1.882569
6	6	0	-3.559611	-2.401931	1.279610
7	1	0	-4.628893	-2.631778	1.437747
8	1	0	-2.987706	-3.190733	1.780045
9	6	0	-3.260873	-2.469233	-0.217619
10	1	0	-3.772535	-1.667616	-0.765295

11	1	0	-3.628421	-3.417116	-0.620547
12	7	0	-1.822204	-2.402774	-0.457738
13	1	0	-1.255648	-1.907410	0.222079
14	6	0	-1.247302	-2.939858	-1.555467
15	6	0	0.229058	-2.895814	-1.636128
16	6	0	1.072208	-3.392948	-2.595728
17	1	0	0.769140	-3.878515	-3.512037
18	6	0	2.397064	-3.154613	-2.134859
19	1	0	3.323722	-3.414865	-2.625805
20	6	0	2.281266	-2.522073	-0.924517
21	6	0	3.326914	-2.061033	0.014115
22	7	0	2.927240	-1.314348	1.066125
23	1	0	1.966120	-0.997916	1.121943
24	6	0	3.877043	-0.813217	2.054810
25	1	0	4.671188	-0.253397	1.546711
26	1	0	4.361819	-1.659881	2.555156
27	6	0	3.183893	0.050744	3.106354
28	1	0	2.441263	-0.553883	3.639651
29	1	0	3.952824	0.346975	3.839891
30	7	0	2.483338	1.210877	2.541014
31	6	0	3.342991	2.297921	2.039577
32	1	0	2.925005	3.254045	2.373737
33	1	0	4.362751	2.229100	2.447173
34	6	0	3.423986	2.317076	0.507142
35	1	0	3.933814	1.422444	0.127646
36	1	0	3.992326	3.188814	0.170727
37	7	0	2.077497	2.395621	-0.042188
38	1	0	1.351602	1.941094	0.502633
39	6	0	1.771880	2.939595	-1.238739
40	6	0	0.332166	2.956555	-1.584058
41	6	0	-0.332759	3.387285	-2.702510
42	1	0	0.123248	3.795643	-3.593007
43	6	0	-1.721906	3.193407	-2.449243
44	1	0	-2.549332	3.422414	-3.105445
45	6	0	-1.818116	2.656461	-1.191865
46	6	0	-2.989894	2.276464	-0.372956
47	7	0	-2.714016	1.744638	0.840976
48	1	0	-1.746033	1.582829	1.086953
49	6	0	-3.745193	1.350554	1.793745
50	1	0	-4.603429	2.013078	1.652935
51	1	0	-3.351715	1.529058	2.798069
52	6	0	-4.221434	-0.097640	1.626121
53	1	0	-4.578871	-0.213718	0.599390
54	1	0	-5.094399	-0.250852	2.290225
55	6	0	-2.922239	-1.259801	3.316529
56	1	0	-2.597930	-0.307085	3.744256
57	1	0	-3.811555	-1.602918	3.878329
58	1	0	-2.116345	-1.984517	3.467423
59	8	0	0.957421	-2.353130	-0.608485
60	8	0	-0.567173	2.503810	-0.655056

61	1	0	1.851500	1.576204	3.247071

***mac*(CH_3)-Fu-CO_2 (DMSO)**

E(RB3LYP) = -1785.67160229 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.739526	0.597215	1.681932
2	8	0	0.886263	4.607669	0.862718
3	8	0	4.901563	0.413630	1.203586
4	8	0	-0.475591	-3.811893	2.453246
5	8	0	-0.459250	0.317644	-1.744357
6	8	0	1.118763	-1.294317	-1.749941
7	7	0	-2.255086	-1.832185	-1.777073
8	1	0	-1.533881	-1.090435	-1.548724
9	6	0	-3.548588	-1.108288	-2.103121
10	1	0	-4.208203	-1.830882	-2.589549
11	1	0	-3.280479	-0.340693	-2.833304
12	6	0	-4.280238	-0.488066	-0.916976
13	1	0	-4.653353	-1.243636	-0.221911
14	1	0	-5.161814	0.020632	-1.329989
15	7	0	-3.430502	0.446557	-0.197446
16	1	0	-2.630131	0.843845	-0.678920
17	6	0	-3.745650	0.942907	1.029877
18	6	0	-2.785327	1.946405	1.534061
19	6	0	-2.693411	2.721919	2.661631
20	1	0	-3.380319	2.720673	3.496168
21	6	0	-1.521196	3.525252	2.505606
22	1	0	-1.133003	4.257553	3.199303
23	6	0	-0.973376	3.185520	1.294721
24	6	0	0.206093	3.629022	0.511526
25	7	0	0.430811	2.889670	-0.593516
26	1	0	-0.152679	2.072876	-0.781411
27	6	0	1.440735	3.191009	-1.599443
28	1	0	2.442946	3.150417	-1.157292
29	1	0	1.291220	4.210189	-1.979252
30	6	0	1.308745	2.196700	-2.762041
31	1	0	0.279096	2.211436	-3.131865
32	1	0	1.954429	2.540602	-3.575669
33	7	0	1.675766	0.813809	-2.445323
34	6	0	3.042517	0.376508	-2.753820
35	1	0	3.002419	-0.658397	-3.104618
36	1	0	3.421816	0.989491	-3.576939
37	6	0	4.039220	0.472056	-1.586107
38	1	0	4.139508	1.502261	-1.226668
39	1	0	5.028527	0.149684	-1.938612

40	7	0	3.572751	-0.379187	-0.500465
41	1	0	2.753384	-0.949214	-0.721702
42	6	0	3.962296	-0.285519	0.787821
43	6	0	3.133404	-1.103407	1.708533
44	6	0	3.146308	-1.380171	3.052501
45	1	0	3.872582	-1.027768	3.771264
46	6	0	2.014227	-2.215740	3.305065
47	1	0	1.703886	-2.627914	4.254814
48	6	0	1.383876	-2.391527	2.098221
49	6	0	0.174117	-3.116993	1.656011
50	7	0	-0.136383	-2.959842	0.341219
51	1	0	0.435581	-2.355959	-0.261575
52	6	0	-1.235575	-3.675425	-0.280674
53	1	0	-1.595929	-4.416340	0.437038
54	1	0	-0.869714	-4.222099	-1.154865
55	6	0	-2.441618	-2.801122	-0.629384
56	1	0	-2.720555	-2.210568	0.243416
57	1	0	-3.280848	-3.444916	-0.908697
58	6	0	-1.745956	-2.497904	-3.024222
59	1	0	-0.706398	-2.781444	-2.872547
60	1	0	-2.365552	-3.368159	-3.246814
61	1	0	-1.802473	-1.778663	-3.841659
62	6	0	0.736374	-0.099714	-1.962260
63	8	0	-1.740568	2.225901	0.703131
64	8	0	2.064169	-1.720205	1.130141

***mac*-Pyr (gas)**

E(RB3LYP) = -1517.98633894 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.573431	-2.125057	-1.410120
2	8	0	3.221055	-3.654027	-1.449431
3	8	0	3.633507	3.543583	-0.940525
4	8	0	-3.274452	2.800106	-1.406213
5	6	0	-3.863225	-1.222037	2.528425
6	1	0	-4.832911	-1.126626	3.034955
7	1	0	-3.163322	-1.628265	3.273007
8	6	0	-4.019235	-2.234423	1.376064
9	1	0	-4.709016	-1.867539	0.613373
10	1	0	-4.432664	-3.175014	1.768000
11	7	0	-2.746184	-2.489534	0.700944
12	1	0	-2.104831	-3.108843	1.182882
13	6	0	-2.638145	-2.442025	-0.681871

14	6	0	-1.301457	-2.749779	-1.231880
15	6	0	-0.969583	-3.143096	-2.522914
16	1	0	-1.682480	-3.273474	-3.324951
17	6	0	0.428985	-3.331461	-2.569842
18	1	0	1.027986	-3.634905	-3.416997
19	6	0	0.939218	-3.028568	-1.313099
20	6	0	2.349920	-3.008250	-0.871440
21	7	0	2.612987	-2.246060	0.249423
22	1	0	1.997816	-1.468021	0.458242
23	6	0	3.974268	-2.072848	0.738855
24	1	0	4.537149	-1.383078	0.094031
25	1	0	4.479975	-3.040586	0.684740
26	6	0	3.947572	-1.577845	2.186571
27	1	0	3.448108	-2.339857	2.796463
28	1	0	4.984638	-1.493404	2.550749
29	7	0	3.215569	-0.307239	2.362143
30	6	0	4.032544	0.922583	2.361212
31	1	0	3.557930	1.639266	3.041620
32	1	0	5.047413	0.726022	2.745403
33	6	0	4.151255	1.582545	0.986521
34	1	0	4.677248	0.928461	0.276363
35	1	0	4.740462	2.499931	1.065562
36	7	0	2.831807	1.941691	0.483147
37	1	0	2.143850	1.200255	0.543896
38	6	0	2.684470	2.894201	-0.506518
39	6	0	1.304849	3.117097	-0.986708
40	6	0	0.891127	3.689120	-2.183743
41	1	0	1.559568	4.077852	-2.939109
42	6	0	-0.519025	3.638364	-2.219762
43	1	0	-1.174930	3.982502	-3.006973
44	6	0	-0.953793	3.055477	-1.035342
45	6	0	-2.346433	2.808914	-0.602564
46	7	0	-2.534277	2.556747	0.745218
47	1	0	-1.846301	2.930611	1.385486
48	6	0	-3.884556	2.368386	1.290191
49	1	0	-4.590481	2.939175	0.678154
50	1	0	-3.885617	2.768686	2.308595
51	6	0	-4.309297	0.897779	1.325281
52	1	0	-4.387205	0.518694	0.294570
53	1	0	-5.312352	0.848628	1.769357
54	1	0	0.167744	2.326664	0.624344
55	1	0	-0.056941	-2.429722	0.466686
56	7	0	0.169898	2.735959	-0.298187
57	7	0	-0.126981	-2.680798	-0.508416
58	1	0	2.700996	-0.349617	3.235872
59	7	0	-3.400316	0.115911	2.171486
60	1	0	-2.499537	0.043820	1.701068

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mac-Pyr-CO_2 (gas)

E(RB3LYP)= -1706.60188417 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	4.884490	-0.614005	-0.950782
2	8	0	0.505493	4.779736	-0.924014
3	8	0	-4.427900	1.416475	-0.899327
4	8	0	-0.284882	-3.931867	-2.358565
5	8	0	0.532805	0.295270	1.331893
6	8	0	-1.107717	-1.157907	1.828952
7	7	0	1.829927	-2.096538	1.657521
8	1	0	1.376662	-1.179220	1.333232
9	6	0	3.009907	-1.760087	2.526310
10	1	0	3.337586	-2.676900	3.027330
11	1	0	2.635640	-1.064226	3.283845
12	6	0	4.163952	-1.140539	1.731194
13	1	0	4.624878	-1.859474	1.049237
14	1	0	4.940252	-0.842183	2.450762
15	7	0	3.705998	-0.031697	0.927535
16	1	0	3.265895	0.747855	1.400405
17	6	0	4.081958	0.138443	-0.401922
18	6	0	3.398445	1.257304	-1.063116
19	6	0	3.801809	2.093188	-2.103099
20	1	0	4.724486	1.992244	-2.658164
21	6	0	2.813092	3.091969	-2.251846
22	1	0	2.814355	3.919280	-2.947964
23	6	0	1.809781	2.826066	-1.324094
24	6	0	0.574812	3.552472	-0.930864
25	7	0	-0.435283	2.728651	-0.495094
26	1	0	-0.328913	1.734982	-0.649385
27	6	0	-1.413382	3.129668	0.503341
28	1	0	-2.422118	2.872741	0.163621
29	1	0	-1.351178	4.218770	0.583331
30	6	0	-1.114372	2.497071	1.882413
31	1	0	-0.045362	2.590319	2.096601
32	1	0	-1.656555	3.067429	2.645662
33	7	0	-1.514909	1.088934	2.037618
34	6	0	-2.762351	0.831866	2.767756
35	1	0	-2.703983	-0.181605	3.171433
36	1	0	-2.810738	1.525063	3.619329
37	6	0	-4.062235	0.978799	1.952021
38	1	0	-4.159348	1.968244	1.498437
39	1	0	-4.912181	0.850502	2.636891
40	7	0	-4.116358	0.001953	0.880106
41	1	0	-3.882690	-0.948567	1.135972
42	6	0	-4.057673	0.330050	-0.457529
43	6	0	-3.429070	-0.714971	-1.297359

44	6	0	-3.533330	-1.033173	-2.648698
45	1	0	-4.221573	-0.574547	-3.345190
46	6	0	-2.586387	-2.047121	-2.916431
47	1	0	-2.391269	-2.535472	-3.861057
48	6	0	-1.908035	-2.316142	-1.728591
49	6	0	-0.761646	-3.208321	-1.483972
50	7	0	-0.246022	-3.165909	-0.201356
51	1	0	-0.636530	-2.537200	0.499672
52	6	0	0.916985	-3.926669	0.182113
53	1	0	1.183563	-4.571147	-0.660736
54	1	0	0.683933	-4.578590	1.039168
55	6	0	2.125551	-3.050815	0.519926
56	1	0	2.440627	-2.452196	-0.336367
57	1	0	2.960879	-3.685044	0.833913
58	6	0	-0.666276	0.037116	1.725681
59	1	0	-2.077444	-1.381971	0.189152
60	1	0	1.597552	1.266332	0.100874
61	7	0	-2.451054	-1.513024	-0.753452
62	7	0	2.183553	1.717661	-0.606946
63	1	0	1.095084	-2.494287	2.253826

***mac*(CH_3)-Pyr (gas)**

E(RB3LYP) = -1557.30105811 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.425112	3.572370	-1.956236
2	8	0	-4.255965	2.780738	-0.458116
3	8	0	-3.071963	-3.017961	-1.971003
4	8	0	3.823352	-2.849107	-1.246951
5	7	0	3.547002	0.502252	1.940967
6	6	0	3.957877	1.879039	1.605010
7	1	0	5.036415	2.027883	1.800789
8	1	0	3.414751	2.561650	2.268162
9	6	0	3.656463	2.280976	0.162922
10	1	0	4.176450	1.635311	-0.558064
11	1	0	4.021858	3.296032	-0.013431
12	7	0	2.218284	2.277985	-0.083317
13	1	0	1.723267	1.467742	0.272294
14	6	0	1.712000	2.920954	-1.195009
15	6	0	0.250994	2.830322	-1.396611
16	6	0	-0.466225	3.086135	-2.556133
17	1	0	-0.021792	3.346483	-3.506554
18	6	0	-1.838684	2.926838	-2.257376

19	1	0	-2.678812	3.034421	-2.929244
20	6	0	-1.940327	2.573987	-0.919800
21	6	0	-3.163689	2.320781	-0.131899
22	7	0	-2.999820	1.561861	1.010943
23	1	0	-2.246279	0.882546	1.019764
24	6	0	-4.171422	1.170969	1.786865
25	1	0	-4.896628	0.640942	1.154391
26	1	0	-4.676647	2.074101	2.143764
27	6	0	-3.753265	0.317225	2.982986
28	1	0	-3.096655	0.912145	3.629289
29	1	0	-4.659002	0.074638	3.565004
30	7	0	-3.009426	-0.896591	2.602041
31	6	0	-3.824205	-2.030041	2.115178
32	1	0	-3.408335	-2.952995	2.536446
33	1	0	-4.865035	-1.950362	2.467117
34	6	0	-3.826289	-2.160473	0.589241
35	1	0	-4.331587	-1.306839	0.117294
36	1	0	-4.375624	-3.058386	0.292411
37	7	0	-2.456304	-2.278117	0.106640
38	1	0	-1.804813	-1.648357	0.562351
39	6	0	-2.193097	-2.646585	-1.197006
40	6	0	-0.768460	-2.596507	-1.589757
41	6	0	-0.217141	-2.551432	-2.861162
42	1	0	-0.788937	-2.528603	-3.778409
43	6	0	1.190661	-2.509297	-2.718529
44	1	0	1.931648	-2.448047	-3.503513
45	6	0	1.476976	-2.526957	-1.361888
46	6	0	2.788511	-2.498556	-0.684822
47	7	0	2.752230	-2.085494	0.637271
48	1	0	2.004500	-1.450426	0.891453
49	6	0	3.981159	-1.922391	1.404207
50	1	0	4.734161	-2.568634	0.947863
51	1	0	3.808613	-2.283848	2.424396
52	6	0	4.503782	-0.480834	1.403636
53	1	0	4.733806	-0.209754	0.369679
54	1	0	5.455702	-0.449054	1.970089
55	6	0	3.389972	0.359780	3.391176
56	1	0	3.027574	-0.641156	3.643097
57	1	0	4.337769	0.526359	3.938255
58	1	0	2.653028	1.083086	3.754568
59	1	0	0.188035	-2.878768	0.273804
60	1	0	-0.448297	2.533610	0.579210
61	7	0	0.272026	-2.541729	-0.677005
62	7	0	-0.655370	2.477999	-0.409843
63	1	0	-2.467313	-1.200800	3.404947

***mac*(CH_3)-Pyr-CO_2 (gas)**

E(RB3LYP) = -1745.90774541 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.435060	0.785424	1.481096
2	8	0	1.032242	4.863806	0.314838
3	8	0	4.614527	0.327028	0.992254
4	8	0	-0.955642	-3.432154	2.753377
5	8	0	-0.435156	0.296051	-1.519708
6	8	0	0.845869	-1.551440	-1.600994
7	7	0	-2.527886	-1.604328	-1.635457
8	1	0	-1.744093	-0.919355	-1.407374
9	6	0	-3.653858	-0.796732	-2.242062
10	1	0	-4.360696	-1.506325	-2.685918
11	1	0	-3.196112	-0.217597	-3.049776
12	6	0	-4.379940	0.129582	-1.265368
13	1	0	-4.939979	-0.417146	-0.503843
14	1	0	-5.119445	0.695154	-1.852564
15	7	0	-3.454037	0.997583	-0.579169
16	1	0	-2.872637	1.605232	-1.142490
17	6	0	-3.545847	1.267111	0.781827
18	6	0	-2.478738	2.149603	1.269192
19	6	0	-2.485423	3.103499	2.284499
20	1	0	-3.300366	3.266403	2.976505
21	6	0	-1.275559	3.827780	2.192998
22	1	0	-0.961062	4.662220	2.804407
23	6	0	-0.540174	3.279975	1.147011
24	6	0	0.724901	3.685448	0.483050
25	7	0	1.445791	2.631086	-0.018519
26	1	0	1.226429	1.702604	0.317853
27	6	0	2.295589	2.726830	-1.191267
28	1	0	3.313392	2.400507	-0.952493
29	1	0	2.341324	3.784711	-1.465928
30	6	0	1.706381	1.911419	-2.361999
31	1	0	0.660505	2.194249	-2.505238
32	1	0	2.254238	2.167791	-3.278191
33	7	0	1.774260	0.454192	-2.190054
34	6	0	2.957200	-0.225681	-2.735377
35	1	0	2.652377	-1.233092	-3.030821
36	1	0	3.262327	0.306807	-3.646386
37	6	0	4.187756	-0.328495	-1.809809
38	1	0	4.536956	0.647468	-1.466067
39	1	0	5.006431	-0.779610	-2.389139
40	7	0	3.892195	-1.123614	-0.633165
41	1	0	3.354380	-1.963965	-0.798964
42	6	0	3.922435	-0.631805	0.654793
43	6	0	2.985275	-1.322187	1.571548
44	6	0	2.955882	-1.490446	2.954183

45	1	0	3.728599	-1.167188	3.637995
46	6	0	1.748851	-2.153850	3.271682
47	1	0	1.396391	-2.449996	4.249949
48	6	0	1.054798	-2.360723	2.079680
49	6	0	-0.284191	-2.932155	1.850522
50	7	0	-0.742753	-2.855702	0.546586
51	1	0	-0.166711	-2.447037	-0.189322
52	6	0	-2.024558	-3.389693	0.159269
53	1	0	-2.486296	-3.805809	1.060575
54	1	0	-1.909375	-4.215790	-0.555738
55	6	0	-2.987773	-2.331884	-0.381438
56	1	0	-3.162803	-1.567732	0.376943
57	1	0	-3.942645	-2.805384	-0.637856
58	6	0	-1.981645	-2.527403	-2.683376
59	1	0	-1.024377	-2.924167	-2.352057
60	1	0	-2.705371	-3.323934	-2.872179
61	1	0	-1.815490	-1.948299	-3.593159
62	6	0	0.682027	-0.293538	-1.756979
63	1	0	1.544251	-1.766330	0.083701
64	1	0	-0.953268	1.639459	-0.146829
65	7	0	1.831954	-1.865771	1.061446
66	7	0	-1.284015	2.266051	0.592910

***mac*-Pyr (DMSO)**

E(RB3LYP) = -1518.03872813 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.530067	-1.996668	-1.484832
2	8	0	3.277084	-3.380227	-1.517198
3	8	0	3.581591	3.318989	-1.130713
4	8	0	-3.321217	2.604685	-1.381205
5	6	0	-3.907654	-1.306002	2.514415
6	1	0	-4.880552	-1.252765	3.019358
7	1	0	-3.202848	-1.746036	3.231759
8	6	0	-4.054724	-2.256612	1.309014
9	1	0	-4.752559	-1.860509	0.569934
10	1	0	-4.450803	-3.219258	1.658974
11	7	0	-2.781140	-2.471384	0.625568
12	1	0	-2.061441	-2.949180	1.154532
13	6	0	-2.609800	-2.323737	-0.719043
14	6	0	-1.247562	-2.556453	-1.250955
15	6	0	-0.892206	-2.870334	-2.560011
16	1	0	-1.587070	-2.983226	-3.380544

17	6	0	0.509853	-3.024011	-2.598138
18	1	0	1.120016	-3.265780	-3.457261
19	6	0	0.995682	-2.781368	-1.316336
20	6	0	2.406600	-2.776122	-0.868280
21	7	0	2.686017	-2.103661	0.278784
22	1	0	2.031034	-1.417474	0.638302
23	6	0	4.034340	-1.992937	0.823325
24	1	0	4.640011	-1.313198	0.209416
25	1	0	4.512174	-2.976036	0.785425
26	6	0	3.964389	-1.512679	2.276527
27	1	0	3.435164	-2.271279	2.863618
28	1	0	4.991065	-1.448655	2.670070
29	7	0	3.242326	-0.238563	2.435145
30	6	0	4.061521	0.985474	2.426891
31	1	0	3.584084	1.710107	3.095540
32	1	0	5.075148	0.797703	2.814625
33	6	0	4.188312	1.623538	1.040033
34	1	0	4.750939	0.976618	0.353857
35	1	0	4.739090	2.565144	1.120306
36	7	0	2.860910	1.899927	0.502647
37	1	0	2.146724	1.236358	0.782864
38	6	0	2.654811	2.715853	-0.563963
39	6	0	1.258632	2.881759	-1.027738
40	6	0	0.825549	3.323608	-2.274732
41	1	0	1.474308	3.624045	-3.085656
42	6	0	-0.584111	3.278094	-2.277760
43	1	0	-1.247799	3.547221	-3.087448
44	6	0	-0.996636	2.826875	-1.026652
45	6	0	-2.389722	2.641683	-0.561520
46	7	0	-2.595124	2.505930	0.778084
47	1	0	-1.843231	2.722984	1.417770
48	6	0	-3.927344	2.324292	1.360859
49	1	0	-4.646423	2.903751	0.774147
50	1	0	-3.892684	2.733049	2.374458
51	6	0	-4.370243	0.858616	1.408418
52	1	0	-4.474258	0.481771	0.378585
53	1	0	-5.365670	0.823836	1.869218
54	1	0	0.155517	2.267316	0.676754
55	1	0	-0.033555	-2.291819	0.476801
56	7	0	0.138577	2.586436	-0.282102
57	7	0	-0.086692	-2.504990	-0.510076
58	1	0	2.711234	-0.269661	3.299242
59	7	0	-3.459203	0.057780	2.231735
60	1	0	-2.544567	0.023193	1.782344

***mac*-Pyr-CO_2 (DMSO)**

E(RB3LYP) = -1706.65515700 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.738054	-0.290840	1.248762
2	8	0	-0.015606	4.821516	1.036830
3	8	0	4.467454	1.010005	1.172182
4	8	0	-0.131427	-4.089265	2.135722
5	8	0	-0.429467	0.354604	-1.378182
6	8	0	1.167355	-1.180060	-1.775084
7	7	0	-2.120172	-1.932503	-1.844142
8	1	0	-1.529969	-1.127836	-1.500390
9	6	0	-3.358823	-1.395227	-2.524509
10	1	0	-3.813526	-2.223257	-3.072792
11	1	0	-3.010031	-0.651359	-3.245157
12	6	0	-4.369868	-0.793218	-1.550369
13	1	0	-4.773778	-1.539530	-0.864220
14	1	0	-5.209298	-0.414543	-2.146851
15	7	0	-3.767553	0.262357	-0.756175
16	1	0	-3.344098	1.031293	-1.261993
17	6	0	-3.963827	0.417373	0.592012
18	6	0	-3.142331	1.482678	1.197452
19	6	0	-3.396953	2.320435	2.282812
20	1	0	-4.274348	2.279124	2.914106
21	6	0	-2.331149	3.244736	2.359441
22	1	0	-2.215452	4.051140	3.070926
23	6	0	-1.434756	2.933297	1.338558
24	6	0	-0.197105	3.603806	0.880982
25	7	0	0.680823	2.791196	0.228161
26	1	0	0.475241	1.799602	0.221839
27	6	0	1.559362	3.236554	-0.849116
28	1	0	2.610552	3.125810	-0.562760
29	1	0	1.371036	4.300851	-1.016397
30	6	0	1.254149	2.448519	-2.137265
31	1	0	0.183192	2.508695	-2.348026
32	1	0	1.787841	2.926960	-2.965117
33	7	0	1.652337	1.034210	-2.104139
34	6	0	2.954208	0.694636	-2.693292
35	1	0	2.883678	-0.311939	-3.111868
36	1	0	3.142897	1.383346	-3.525054
37	6	0	4.168573	0.759649	-1.743775
38	1	0	4.261739	1.732670	-1.257879
39	1	0	5.075406	0.600257	-2.341566
40	7	0	4.062227	-0.252977	-0.702779
41	1	0	3.765979	-1.166940	-1.021388
42	6	0	3.997464	-0.006355	0.638241
43	6	0	3.249746	-1.033359	1.398936
44	6	0	3.278922	-1.442194	2.732546

45	1	0	3.976552	-1.096796	3.483673
46	6	0	2.245783	-2.392246	2.900833
47	1	0	1.986035	-2.919603	3.808550
48	6	0	1.597257	-2.531503	1.671227
49	6	0	0.407243	-3.330378	1.312706
50	7	0	-0.050888	-3.174606	0.035167
51	1	0	0.405466	-2.523531	-0.608270
52	6	0	-1.211275	-3.870513	-0.483743
53	1	0	-1.529865	-4.605098	0.259053
54	1	0	-0.937582	-4.417107	-1.395452
55	6	0	-2.401048	-2.951820	-0.762409
56	1	0	-2.692488	-2.403265	0.133605
57	1	0	-3.245043	-3.554799	-1.106432
58	6	0	0.756531	0.030844	-1.745011
59	1	0	1.914356	-1.510002	-0.179560
60	1	0	-1.466597	1.377888	-0.121728
61	7	0	2.235665	-1.714070	0.776410
62	7	0	-1.947272	1.865805	0.641401
63	1	0	-1.548721	-2.369894	-2.575567

***mac*(CH_3)-Pyr (DMSO)**

E(RB3LYP)= -1557.34602097 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.963756	3.851998	-1.997265
2	8	0	-4.593863	2.282309	-0.725244
3	8	0	-2.705119	-2.486558	-1.942753
4	8	0	4.141196	-3.184080	-0.931481
5	7	0	3.449006	0.937910	1.856655
6	6	0	3.568722	2.396590	1.685324
7	1	0	4.572770	2.753567	1.976881
8	1	0	2.851575	2.874200	2.361458
9	6	0	3.278085	2.873961	0.263254
10	1	0	3.960072	2.418358	-0.465625
11	1	0	3.438382	3.955201	0.212544
12	7	0	1.890805	2.595154	-0.098614
13	1	0	1.460643	1.799319	0.359447
14	6	0	1.329025	3.117666	-1.221111
15	6	0	-0.095098	2.810581	-1.474988
16	6	0	-0.785211	2.912505	-2.678649
17	1	0	-0.341868	3.180116	-3.627804
18	6	0	-2.135643	2.586534	-2.426550
19	1	0	-2.945638	2.548378	-3.141848

20	6	0	-2.250402	2.288680	-1.072808
21	6	0	-3.472958	1.933089	-0.318365
22	7	0	-3.299563	1.239946	0.837530
23	1	0	-2.445405	0.709337	0.985421
24	6	0	-4.426398	0.815334	1.661085
25	1	0	-5.075762	0.131980	1.097702
26	1	0	-5.033693	1.687976	1.921618
27	6	0	-3.907997	0.152835	2.940082
28	1	0	-3.381885	0.903710	3.539941
29	1	0	-4.779528	-0.188317	3.523930
30	7	0	-2.959021	-0.934281	2.667886
31	6	0	-3.550200	-2.218198	2.262463
32	1	0	-3.010144	-3.026055	2.771987
33	1	0	-4.599952	-2.293962	2.587238
34	6	0	-3.514663	-2.479999	0.752634
35	1	0	-4.002472	-1.675274	0.197645
36	1	0	-4.071605	-3.403824	0.541263
37	7	0	-2.142570	-2.596979	0.265032
38	1	0	-1.449151	-2.924192	0.926258
39	6	0	-1.838568	-2.600460	-1.059955
40	6	0	-0.408297	-2.732913	-1.416439
41	6	0	0.138050	-3.209584	-2.604606
42	1	0	-0.432751	-3.532514	-3.464207
43	6	0	1.542446	-3.213473	-2.458736
44	1	0	2.276527	-3.525609	-3.188667
45	6	0	1.835291	-2.715668	-1.192592
46	6	0	3.163848	-2.506390	-0.572504
47	7	0	3.234210	-1.559401	0.398917
48	1	0	2.471078	-0.904811	0.529627
49	6	0	4.439208	-1.265746	1.165283
50	1	0	5.295782	-1.685009	0.633164
51	1	0	4.387530	-1.763053	2.142061
52	6	0	4.632134	0.245217	1.319990
53	1	0	4.854471	0.662709	0.333888
54	1	0	5.517866	0.420008	1.958978
55	6	0	3.215754	0.601552	3.266352
56	1	0	3.057479	-0.474175	3.381466
57	1	0	4.061673	0.896553	3.914336
58	1	0	2.314412	1.111930	3.618282
59	1	0	0.544970	-2.062610	0.363652
60	1	0	-0.822252	2.440099	0.485117
61	7	0	0.638549	-2.431617	-0.573208
62	7	0	-0.995355	2.402923	-0.511913
63	1	0	-2.376068	-1.071653	3.487223

***mac*(CH_3)-Pyr-CO_2 (DMSO)**

E(RB3LYP) = -1745.96046627 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.177784	1.048972	1.759279
2	8	0	1.549335	4.777458	0.508864
3	8	0	4.585421	-0.133357	1.191517
4	8	0	-1.307803	-3.571860	2.502009
5	8	0	-0.357710	0.402404	-1.465742
6	8	0	0.790829	-1.528852	-1.608710
7	7	0	-2.740497	-1.293652	-1.708960
8	1	0	-1.914622	-0.709069	-1.423833
9	6	0	-3.838955	-0.346466	-2.154247
10	1	0	-4.624171	-0.956108	-2.608447
11	1	0	-3.396533	0.278960	-2.933081
12	6	0	-4.430604	0.519727	-1.043643
13	1	0	-4.947007	-0.067082	-0.283731
14	1	0	-5.182254	1.166224	-1.514579
15	7	0	-3.403387	1.305893	-0.385176
16	1	0	-2.846635	1.912523	-0.975501
17	6	0	-3.341753	1.506647	0.969032
18	6	0	-2.179552	2.305564	1.402487
19	6	0	-2.055014	3.212387	2.454405
20	1	0	-2.812462	3.415470	3.199477
21	6	0	-0.796909	3.841270	2.320499
22	1	0	-0.382783	4.615615	2.952049
23	6	0	-0.168731	3.283444	1.208976
24	6	0	1.099393	3.621345	0.524235
25	7	0	1.677068	2.582085	-0.139946
26	1	0	1.302447	1.657750	0.033160
27	6	0	2.446391	2.715955	-1.371765
28	1	0	3.490417	2.425453	-1.213515
29	1	0	2.437665	3.769894	-1.663207
30	6	0	1.796003	1.864848	-2.478449
31	1	0	0.755127	2.171304	-2.601448
32	1	0	2.321741	2.058305	-3.420488
33	7	0	1.825434	0.420170	-2.218268
34	6	0	3.000563	-0.319464	-2.699057
35	1	0	2.669597	-1.305631	-3.034665
36	1	0	3.396572	0.207601	-3.574440
37	6	0	4.162328	-0.495211	-1.698281
38	1	0	4.508811	0.457980	-1.294508
39	1	0	5.003965	-0.950232	-2.237293
40	7	0	3.757675	-1.336852	-0.580824
41	1	0	3.171776	-2.123191	-0.830937
42	6	0	3.807442	-0.986485	0.737155
43	6	0	2.796886	-1.672326	1.575095
44	6	0	2.721918	-1.960124	2.938664

45	1	0	3.498973	-1.772245	3.667450
46	6	0	1.458847	-2.551101	3.171881
47	1	0	1.068821	-2.905204	4.116422
48	6	0	0.783716	-2.597138	1.949127
49	6	0	-0.584797	-3.055862	1.633469
50	7	0	-0.991131	-2.873415	0.340904
51	1	0	-0.369219	-2.438070	-0.344612
52	6	0	-2.285351	-3.304350	-0.149485
53	1	0	-2.789804	-3.837441	0.659758
54	1	0	-2.157279	-4.013387	-0.974271
55	6	0	-3.208832	-2.152987	-0.547928
56	1	0	-3.347007	-1.483738	0.301385
57	1	0	-4.179165	-2.562056	-0.843115
58	6	0	-2.287193	-2.100000	-2.893733
59	1	0	-1.360591	-2.613595	-2.645637
60	1	0	-3.071332	-2.809041	-3.163127
61	1	0	-2.101164	-1.413518	-3.719982
62	6	0	0.700289	-0.259978	-1.751467
63	1	0	1.363909	-1.871632	0.023733
64	1	0	-0.800185	1.736595	-0.126322
65	7	0	1.621050	-2.076048	0.999615
66	7	0	-1.023700	2.354857	0.663194

***mac*-Tf (gas)**

E(RB3LYP) = -2203.65398613 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.824644	-2.231066	-1.436051
2	8	0	3.141598	-3.508849	-1.778327
3	8	0	3.842440	3.434368	-0.956892
4	8	0	-3.202877	3.157048	-1.609955
5	6	0	-4.534541	-1.058995	2.385471
6	1	0	-5.555127	-0.913599	2.763028
7	1	0	-3.936272	-1.412368	3.237583
8	6	0	-4.572451	-2.159263	1.303979
9	1	0	-5.194592	-1.867604	0.455405
10	1	0	-5.004093	-3.076119	1.730976
11	7	0	-3.243689	-2.431835	0.767965
12	1	0	-2.545127	-2.799639	1.402410
13	6	0	-2.969701	-2.434535	-0.577085
14	6	0	-1.551012	-2.672989	-0.964029
15	6	0	-1.128025	-3.047174	-2.218872
16	1	0	-1.826579	-3.204941	-3.032530

17	6	0	0.281016	-3.188094	-2.317880
18	1	0	0.815129	-3.473039	-3.217025
19	6	0	0.941218	-2.906139	-1.143728
20	6	0	2.422417	-2.915073	-0.976243
21	7	0	2.917631	-2.241941	0.106271
22	1	0	2.329013	-1.585416	0.606135
23	6	0	4.347383	-2.097801	0.334934
24	1	0	4.772257	-1.342500	-0.340650
25	1	0	4.831414	-3.048356	0.093088
26	6	0	4.606993	-1.737116	1.800219
27	1	0	4.246802	-2.564507	2.422827
28	1	0	5.695551	-1.658970	1.956108
29	7	0	3.914449	-0.508883	2.234052
30	6	0	4.705604	0.734147	2.206653
31	1	0	4.298762	1.401703	2.975144
32	1	0	5.763013	0.545403	2.458895
33	6	0	4.653448	1.464075	0.863013
34	1	0	5.116723	0.863148	0.067701
35	1	0	5.224387	2.395020	0.925511
36	7	0	3.278106	1.795472	0.523413
37	1	0	2.579383	1.113801	0.794749
38	6	0	2.978022	2.756279	-0.402485
39	6	0	1.535545	2.965316	-0.712305
40	6	0	1.062648	3.621850	-1.825725
41	1	0	1.733992	4.054936	-2.558279
42	6	0	-0.353946	3.652177	-1.902250
43	1	0	-0.923835	4.109454	-2.702784
44	6	0	-0.971682	3.031344	-0.840758
45	6	0	-2.449628	2.925660	-0.666587
46	7	0	-2.897843	2.557772	0.574716
47	1	0	-2.245328	2.548356	1.347451
48	6	0	-4.318303	2.425738	0.893427
49	1	0	-4.877401	2.952998	0.116200
50	1	0	-4.497507	2.914542	1.857316
51	6	0	-4.774985	0.964684	0.969430
52	1	0	-4.717390	0.512415	-0.033414
53	1	0	-5.829502	0.954807	1.275212
54	16	0	-0.190555	-2.479373	0.117955
55	16	0	0.212574	2.385378	0.273116
56	1	0	3.557920	-0.645878	3.174199
57	7	0	-4.000921	0.238488	1.982687
58	1	0	-3.050302	0.110203	1.638628

***mac*-Tf-CO_2 (gas)**

E(RB3LYP) = -2392.21448599 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-5.026458	-0.328070	0.767932
2	8	0	0.646678	4.076658	1.565759
3	8	0	4.567498	1.296742	0.636840
4	8	0	-0.669954	-2.908401	2.853519
5	8	0	-0.348842	0.285561	-1.498914
6	8	0	0.797320	-1.581201	-1.995735
7	7	0	-2.046196	-1.823581	-1.483137
8	1	0	-1.550961	-0.906097	-1.237097
9	6	0	-3.115680	-1.556770	-2.506270
10	1	0	-3.374159	-2.511112	-2.977409
11	1	0	-2.649731	-0.916581	-3.262110
12	6	0	-4.387977	-0.901603	-1.939717
13	1	0	-4.918565	-1.560991	-1.248475
14	1	0	-5.057935	-0.718624	-2.790652
15	7	0	-4.101689	0.323886	-1.223290
16	1	0	-3.420850	0.940824	-1.649949
17	6	0	-4.312518	0.453126	0.143307
18	6	0	-3.487593	1.497736	0.796613
19	6	0	-3.056962	1.460410	2.107831
20	1	0	-3.516525	0.815385	2.849053
21	6	0	-1.873820	2.224642	2.332254
22	1	0	-1.335424	2.251187	3.273401
23	6	0	-1.391888	2.815872	1.186643
24	6	0	0.010944	3.284580	0.876396
25	7	0	0.453549	2.652821	-0.244659
26	1	0	-0.080531	1.854092	-0.596417
27	6	0	1.774612	2.750778	-0.846007
28	1	0	2.558153	2.404006	-0.162820
29	1	0	1.988305	3.801238	-1.081909
30	6	0	1.775279	1.938747	-2.157369
31	1	0	0.877020	2.197388	-2.733322
32	1	0	2.637438	2.267986	-2.744410
33	7	0	1.879758	0.466963	-2.047504
34	6	0	3.049505	-0.121194	-2.711111
35	1	0	2.877484	-1.198221	-2.768805
36	1	0	3.110833	0.254029	-3.746961
37	6	0	4.413561	0.159513	-2.038182
38	1	0	4.576997	1.224693	-1.857039
39	1	0	5.202473	-0.179094	-2.721494
40	7	0	4.555984	-0.524985	-0.754256
41	1	0	4.290986	-1.502013	-0.798625
42	6	0	4.258960	0.127251	0.429818
43	6	0	3.394581	-0.624660	1.382648
44	6	0	2.794698	-0.128474	2.523316
45	1	0	3.113506	0.798434	2.987109
46	6	0	1.650807	-0.874662	2.921358

47	1	0	0.993842	-0.601100	3.739597
48	6	0	1.374339	-1.926803	2.071832
49	6	0	0.088443	-2.659913	1.920146
50	7	0	-0.192531	-2.977953	0.607528
51	1	0	0.364447	-2.561263	-0.140826
52	6	0	-1.430068	-3.608970	0.211785
53	1	0	-1.840898	-4.132202	1.079862
54	1	0	-1.216540	-4.355329	-0.565550
55	6	0	-2.498610	-2.631091	-0.287033
56	1	0	-2.797798	-1.933285	0.496250
57	1	0	-3.381790	-3.200820	-0.591174
58	6	0	0.732509	-0.322346	-1.849576
59	16	0	-2.482760	2.569548	-0.143616
60	16	0	2.585237	-2.066145	0.841895
61	1	0	-1.240199	-2.274373	-1.952753

***mac*(CH_3)-Tf (gas)**

E(RB3LYP) = -2242.96497688 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.278625	3.934546	-2.089628
2	8	0	-4.503675	3.159724	-0.389005
3	8	0	-2.837473	-3.575371	-2.044923
4	8	0	4.102325	-3.413664	-0.728167
5	7	0	4.149300	0.887669	1.579076
6	6	0	4.468446	2.195286	0.975766
7	1	0	5.560909	2.368762	0.962792
8	1	0	4.027946	2.976341	1.604782
9	6	0	3.918978	2.363987	-0.440614
10	1	0	4.295333	1.580307	-1.112319
11	1	0	4.248432	3.320403	-0.854014
12	7	0	2.462821	2.374329	-0.438619
13	1	0	2.002292	1.677503	0.133249
14	6	0	1.744388	3.177549	-1.278434
15	6	0	0.257655	3.128646	-1.174994
16	6	0	-0.591343	3.770199	-2.048401
17	1	0	-0.213558	4.341143	-2.888472
18	6	0	-1.962044	3.606752	-1.724897
19	1	0	-2.788031	4.032945	-2.282401
20	6	0	-2.169996	2.836682	-0.603290
21	6	0	-3.512890	2.515938	-0.044096
22	7	0	-3.584055	1.497698	0.865599
23	1	0	-2.821929	0.835348	0.950946

24	6	0	-4.863353	1.070276	1.412188
25	1	0	-5.479059	0.599139	0.632574
26	1	0	-5.412946	1.954917	1.747797
27	6	0	-4.648984	0.120046	2.589593
28	1	0	-4.104448	0.652385	3.378317
29	1	0	-5.639418	-0.151428	2.994464
30	7	0	-3.857189	-1.068039	2.233770
31	6	0	-4.574186	-2.126134	1.492775
32	1	0	-4.321511	-3.095758	1.937692
33	1	0	-5.664634	-2.000789	1.581551
34	6	0	-4.196902	-2.167446	0.007772
35	1	0	-4.528882	-1.254104	-0.505163
36	1	0	-4.682752	-3.012990	-0.486533
37	7	0	-2.759124	-2.333009	-0.132391
38	1	0	-2.192010	-1.791943	0.509233
39	6	0	-2.183449	-3.016128	-1.165070
40	6	0	-0.693011	-3.073492	-1.181221
41	6	0	0.057122	-3.615882	-2.199816
42	1	0	-0.407530	-4.039237	-3.082732
43	6	0	1.455206	-3.558235	-1.962460
44	1	0	2.215866	-3.933560	-2.637311
45	6	0	1.780382	-2.965293	-0.763814
46	6	0	3.165205	-2.776158	-0.249638
47	7	0	3.314150	-1.879042	0.775251
48	1	0	2.560321	-1.237482	0.986132
49	6	0	4.605859	-1.582954	1.375191
50	1	0	5.325066	-2.284381	0.946242
51	1	0	4.557463	-1.779425	2.453452
52	6	0	5.072134	-0.151441	1.092975
53	1	0	5.175849	-0.039765	0.009636
54	1	0	6.080196	-0.015839	1.533209
55	6	0	4.160251	0.978251	3.041978
56	1	0	3.872332	0.022006	3.487932
57	1	0	5.153985	1.256491	3.442380
58	1	0	3.434350	1.729387	3.368181
59	16	0	-0.647533	2.317223	0.083604
60	16	0	0.339420	-2.494350	0.105869
61	1	0	-3.460377	-1.458158	3.082819

***mac*(CH_3)-Tf-CO_2 (gas)**

E(RB3LYP) = -2431.51792819 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	8	0	4.822406	0.399917	-1.297389
2	8	0	-1.407601	4.156874	-1.075722
3	8	0	-5.021324	0.513417	-0.941809
4	8	0	1.182666	-2.652604	-2.952679
5	8	0	0.298701	0.174522	1.756122
6	8	0	-1.091336	-1.600216	1.649668
7	7	0	2.334365	-1.768013	1.630415
8	1	0	1.594262	-1.009112	1.469743
9	6	0	3.537921	-1.142078	2.315281
10	1	0	4.073285	-1.959333	2.810109
11	1	0	3.124120	-0.489864	3.090923
12	6	0	4.525580	-0.369219	1.434689
13	1	0	4.995322	-0.995272	0.672426
14	1	0	5.329957	-0.034365	2.106758
15	7	0	3.892500	0.744963	0.768741
16	1	0	3.116549	1.180459	1.252286
17	6	0	4.020987	0.999972	-0.587880
18	6	0	3.001944	1.953146	-1.094496
19	6	0	2.380017	1.900181	-2.323562
20	1	0	2.777294	1.321233	-3.150564
21	6	0	1.104907	2.544866	-2.332902
22	1	0	0.426529	2.539788	-3.179073
23	6	0	0.755678	3.058079	-1.105904
24	6	0	-0.601977	3.397178	-0.548494
25	7	0	-0.802623	2.708430	0.613122
26	1	0	-0.164737	1.947066	0.844809
27	6	0	-1.991087	2.767872	1.449240
28	1	0	-2.885722	2.483434	0.881724
29	1	0	-2.139378	3.798400	1.798189
30	6	0	-1.773311	1.839907	2.660321
31	1	0	-0.780359	2.034367	3.081953
32	1	0	-2.509790	2.103478	3.426555
33	7	0	-1.911502	0.404230	2.396888
34	6	0	-3.171295	-0.223656	2.812617
35	1	0	-2.964585	-1.277816	3.015063
36	1	0	-3.494230	0.236378	3.755591
37	6	0	-4.330298	-0.128045	1.801528
38	1	0	-4.586578	0.908211	1.555174
39	1	0	-5.224757	-0.586178	2.247477
40	7	0	-3.933148	-0.820222	0.585192
41	1	0	-3.079705	-1.360674	0.703444
42	6	0	-4.186426	-0.346152	-0.678817
43	6	0	-3.211751	-0.891749	-1.679574
44	6	0	-2.550741	-0.151330	-2.634949
45	1	0	-2.899054	0.825698	-2.952647
46	6	0	-1.299273	-0.723811	-3.014640
47	1	0	-0.582966	-0.244095	-3.672651
48	6	0	-1.017797	-1.888883	-2.336402
49	6	0	0.318513	-2.496711	-2.094082
50	7	0	0.510169	-2.809053	-0.760588

51	1	0	-0.148388	-2.456069	-0.061451
52	6	0	1.733416	-3.411837	-0.290163
53	1	0	2.238972	-3.846482	-1.158489
54	1	0	1.499244	-4.231290	0.398877
55	6	0	2.744740	-2.444583	0.333960
56	1	0	2.990270	-1.653700	-0.375991
57	1	0	3.658482	-3.004682	0.563716
58	6	0	1.683580	-2.709615	2.604217
59	1	0	0.675200	-2.934304	2.257988
60	1	0	2.300289	-3.606114	2.704605
61	1	0	1.605681	-2.198089	3.565107
62	6	0	-0.853456	-0.384035	1.912830
63	16	0	2.062016	2.899980	0.028635
64	16	0	-2.359568	-2.371585	-1.341789

***mac*-Tf (DMSO)**

E(RB3LYP) = -2203.69291840 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.613741	-2.074805	-1.638875
2	8	0	3.357653	-3.362961	-1.607854
3	8	0	3.640334	3.328463	-1.282907
4	8	0	-3.415949	2.786961	-1.462560
5	6	0	-4.576021	-1.333614	2.280167
6	1	0	-5.616405	-1.274888	2.623726
7	1	0	-3.998636	-1.785790	3.096844
8	6	0	-4.536993	-2.273455	1.058312
9	1	0	-5.121110	-1.875799	0.227045
10	1	0	-4.973176	-3.241552	1.338992
11	7	0	-3.174477	-2.469953	0.570470
12	1	0	-2.499029	-2.841389	1.228786
13	6	0	-2.811346	-2.342896	-0.732716
14	6	0	-1.367866	-2.533384	-1.051507
15	6	0	-0.872458	-2.857858	-2.295740
16	1	0	-1.514934	-3.004858	-3.156129
17	6	0	0.540258	-2.982605	-2.320028
18	1	0	1.118029	-3.231174	-3.202673
19	6	0	1.128448	-2.736247	-1.098501
20	6	0	2.596073	-2.754844	-0.839244
21	7	0	3.035804	-2.092681	0.256758
22	1	0	2.420031	-1.453859	0.749262
23	6	0	4.446420	-1.991365	0.611094
24	1	0	4.964972	-1.320417	-0.086072

25	1	0	4.908521	-2.978318	0.513811
26	6	0	4.582013	-1.501797	2.056480
27	1	0	4.135679	-2.252906	2.717428
28	1	0	5.654351	-1.443465	2.301138
29	7	0	3.896162	-0.223288	2.306056
30	6	0	4.702940	0.998203	2.146728
31	1	0	4.335728	1.735787	2.868651
32	1	0	5.765481	0.816123	2.372889
33	6	0	4.609450	1.610242	0.745122
34	1	0	5.064756	0.952977	-0.007189
35	1	0	5.157600	2.556532	0.722005
36	7	0	3.213441	1.865950	0.411702
37	1	0	2.546060	1.233769	0.841308
38	6	0	2.830550	2.692798	-0.589302
39	6	0	1.367028	2.829115	-0.838379
40	6	0	0.809775	3.337796	-1.991638
41	1	0	1.413146	3.696162	-2.817434
42	6	0	-0.608005	3.323999	-1.981608
43	1	0	-1.230072	3.674819	-2.796604
44	6	0	-1.139561	2.817102	-0.815377
45	6	0	-2.598312	2.689424	-0.535744
46	7	0	-2.970250	2.466569	0.751523
47	1	0	-2.271116	2.504255	1.482203
48	6	0	-4.366190	2.303647	1.161811
49	1	0	-4.989034	2.901718	0.491409
50	1	0	-4.457629	2.704721	2.175277
51	6	0	-4.835884	0.845424	1.135397
52	1	0	-4.785921	0.472543	0.099506
53	1	0	-5.890503	0.825525	1.438104
54	16	0	-0.074931	-2.363899	0.110299
55	16	0	0.126917	2.339181	0.288561
56	1	0	3.507152	-0.238311	3.243085
57	7	0	-4.075351	0.027679	2.085137
58	1	0	-3.101320	-0.016016	1.786940

***mac*-Tf-CO_2 (DMSO)**

E(RB3LYP) = -2392.26167741 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.838866	0.075806	1.185095
2	8	0	1.001261	4.221033	0.894843
3	8	0	4.511931	1.147996	0.980770
4	8	0	-1.169411	-2.711135	2.751164

5	8	0	-0.046301	0.017845	-1.649110
6	8	0	1.104740	-1.904204	-1.838121
7	7	0	-2.448721	-1.815239	-1.618704
8	1	0	-1.766178	-1.045753	-1.416360
9	6	0	-3.652587	-1.333559	-2.416919
10	1	0	-4.050769	-2.216848	-2.922218
11	1	0	-3.260607	-0.651513	-3.174856
12	6	0	-4.787047	-0.677411	-1.613871
13	1	0	-5.168921	-1.328714	-0.826676
14	1	0	-5.605493	-0.522510	-2.325905
15	7	0	-4.404293	0.584547	-1.005668
16	1	0	-4.039795	1.288903	-1.635928
17	6	0	-4.268537	0.782465	0.346042
18	6	0	-3.265507	1.805596	0.732082
19	6	0	-2.897507	2.222071	1.997378
20	1	0	-3.479577	1.998025	2.884521
21	6	0	-1.638868	2.887250	2.020533
22	1	0	-1.154335	3.235147	2.926416
23	6	0	-1.042064	2.946072	0.776849
24	6	0	0.367373	3.279755	0.390347
25	7	0	0.842812	2.435458	-0.549132
26	1	0	0.309093	1.593797	-0.808047
27	6	0	2.129639	2.526131	-1.225193
28	1	0	2.950796	2.309191	-0.532693
29	1	0	2.270044	3.545797	-1.605832
30	6	0	2.137474	1.544014	-2.410190
31	1	0	1.248351	1.724906	-3.025946
32	1	0	3.009850	1.782170	-3.026352
33	7	0	2.216806	0.111711	-2.070954
34	6	0	3.457920	-0.557438	-2.470403
35	1	0	3.274402	-1.632897	-2.435859
36	1	0	3.699661	-0.298836	-3.513607
37	6	0	4.703784	-0.220312	-1.616041
38	1	0	4.863546	0.856321	-1.526143
39	1	0	5.582574	-0.643309	-2.115737
40	7	0	4.603595	-0.775394	-0.262049
41	1	0	4.325915	-1.750387	-0.263004
42	6	0	4.163699	-0.025004	0.802802
43	6	0	3.122921	-0.653173	1.660801
44	6	0	2.389780	-0.035405	2.657710
45	1	0	2.687697	0.905875	3.105540
46	6	0	1.158316	-0.689399	2.930314
47	1	0	0.409312	-0.313799	3.618699
48	6	0	0.952057	-1.793796	2.125344
49	6	0	-0.329457	-2.506480	1.865081
50	7	0	-0.504625	-2.862058	0.559004
51	1	0	0.142303	-2.528732	-0.166551
52	6	0	-1.696872	-3.542813	0.092857
53	1	0	-2.107752	-4.135023	0.914363
54	1	0	-1.410844	-4.235262	-0.706292

55	6	0	-2.813885	-2.613982	-0.386332
56	1	0	-3.105189	-1.906189	0.390181
57	1	0	-3.679120	-3.224316	-0.655741
58	6	0	1.036182	-0.640582	-1.855129
59	16	0	-2.068530	2.269509	-0.439069
60	16	0	2.316083	-2.090943	1.108299
61	1	0	-1.912558	-2.419004	-2.252626

***mac*(CH_3)-Tf (DMSO)**

E(RB3LYP) = -2243.00115618 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.553451	-3.785023	-2.036700
2	8	0	4.324711	-3.112491	-0.775806
3	8	0	3.124737	3.405137	-1.866480
4	8	0	-3.850956	3.624819	-0.914153
5	7	0	-4.096223	-0.661407	1.679023
6	6	0	-4.451383	-2.052984	1.350955
7	1	0	-5.533978	-2.233085	1.480073
8	1	0	-3.931223	-2.708167	2.057719
9	6	0	-4.055512	-2.469249	-0.065276
10	1	0	-4.553812	-1.853600	-0.824999
11	1	0	-4.371905	-3.502081	-0.235575
12	7	0	-2.607158	-2.400552	-0.230680
13	1	0	-2.125981	-1.697519	0.319770
14	6	0	-1.957699	-3.081461	-1.204908
15	6	0	-0.471728	-2.984252	-1.244352
16	6	0	0.306881	-3.356070	-2.319164
17	1	0	-0.121123	-3.720572	-3.245646
18	6	0	1.697052	-3.213851	-2.079705
19	1	0	2.470037	-3.452604	-2.800932
20	6	0	1.984356	-2.730704	-0.821663
21	6	0	3.356869	-2.510101	-0.284791
22	7	0	3.482783	-1.648066	0.751351
23	1	0	2.722600	-1.020089	0.990814
24	6	0	4.768719	-1.339273	1.365613
25	1	0	5.414352	-0.811277	0.651666
26	1	0	5.276589	-2.273661	1.624758
27	6	0	4.552118	-0.507971	2.631793
28	1	0	3.989295	-1.107430	3.355851
29	1	0	5.539999	-0.296560	3.072755
30	7	0	3.783188	0.720755	2.385064
31	6	0	4.540128	1.857181	1.829699

32	1	0	4.220763	2.769402	2.345647
33	1	0	5.620481	1.743664	2.005604
34	6	0	4.310097	2.049667	0.326056
35	1	0	4.702202	1.198398	-0.245710
36	1	0	4.834043	2.945149	-0.018620
37	7	0	2.885998	2.215435	0.062486
38	1	0	2.270271	1.688027	0.672407
39	6	0	2.395278	2.874504	-1.013102
40	6	0	0.912987	2.964481	-1.143048
41	6	0	0.252668	3.483866	-2.235879
42	1	0	0.779363	3.853648	-3.107711
43	6	0	-1.158213	3.483832	-2.091815
44	1	0	-1.850172	3.854760	-2.839034
45	6	0	-1.580408	2.953453	-0.892548
46	6	0	-2.998656	2.855719	-0.443918
47	7	0	-3.278382	1.908863	0.485155
48	1	0	-2.574915	1.223301	0.735391
49	6	0	-4.587869	1.738902	1.102862
50	1	0	-5.301035	2.351164	0.547790
51	1	0	-4.557992	2.122366	2.130191
52	6	0	-5.048536	0.279789	1.068718
53	1	0	-5.192024	-0.007151	0.023167
54	1	0	-6.036129	0.219446	1.564484
55	6	0	-4.009214	-0.482714	3.133304
56	1	0	-3.675033	0.529644	3.375391
57	1	0	-4.978252	-0.655871	3.637193
58	1	0	-3.274973	-1.182745	3.542555
59	16	0	0.521694	-2.461164	0.093730
60	16	0	-0.221715	2.469812	0.089853
61	1	0	3.339506	1.003753	3.253012

***mac*(CH_3)-Tf -CO_2 (DMSO)**

E(RB3LYP) = -2431.59659290 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.337248	2.162085	-2.018460redwds
2	8	0	-3.662299	2.765023	-1.785076
3	8	0	-3.323333	-2.614409	-2.203416
4	8	0	3.704340	-2.000470	-1.841163
5	8	0	-2.094201	0.924487	2.679143
6	8	0	-2.024359	-1.334207	2.517237
7	7	0	4.302693	0.087947	1.885056
8	1	0	3.335192	0.060520	1.532307

9	6	0	4.754282	1.538375	1.845198
10	1	0	5.829900	1.544883	2.032350
11	1	0	4.258717	2.032578	2.683512
12	6	0	4.443925	2.257338	0.537501
13	1	0	4.951373	1.808713	-0.316562
14	1	0	4.836264	3.277490	0.641437
15	7	0	3.015148	2.272358	0.243107
16	1	0	2.411218	2.686748	0.945861
17	6	0	2.572044	2.294877	-1.057942
18	6	0	1.113876	2.466406	-1.272131
19	6	0	0.545822	2.883396	-2.457696
20	1	0	1.137550	3.130306	-3.331465
21	6	0	-0.867190	2.953148	-2.400238
22	1	0	-1.500856	3.251339	-3.226756
23	6	0	-1.384398	2.582323	-1.176252
24	6	0	-2.847291	2.491292	-0.884414
25	7	0	-3.226829	2.092806	0.345083
26	1	0	-2.555031	1.843057	1.080962
27	6	0	-4.623435	1.792772	0.655509
28	1	0	-5.050783	1.209721	-0.168387
29	1	0	-5.207229	2.720554	0.732392
30	6	0	-4.724407	1.025089	1.981774
31	1	0	-4.384461	1.669463	2.797729
32	1	0	-5.781987	0.799590	2.156436
33	7	0	-3.965613	-0.223149	2.033663
34	6	0	-4.631390	-1.489665	1.735376
35	1	0	-4.274588	-2.246103	2.441137
36	1	0	-5.706573	-1.364066	1.900414
37	6	0	-4.439060	-2.005288	0.301006
38	1	0	-4.846058	-1.293681	-0.426956
39	1	0	-4.993569	-2.946200	0.181548
40	7	0	-3.020057	-2.214847	0.018464
41	1	0	-2.391739	-2.045307	0.813556
42	6	0	-2.567126	-2.444019	-1.229223
43	6	0	-1.087192	-2.474389	-1.438507
44	6	0	-0.476242	-2.688576	-2.656883
45	1	0	-1.042601	-2.890116	-3.558270
46	6	0	0.936956	-2.601995	-2.600444
47	1	0	1.594054	-2.736369	-3.451881
48	6	0	1.409772	-2.328059	-1.334007
49	6	0	2.840935	-2.174405	-0.974592
50	7	0	3.155818	-2.218263	0.360180
51	1	0	2.466985	-2.592680	1.001365
52	6	0	4.542983	-2.210423	0.812640
53	1	0	5.172147	-2.721811	0.077563
54	1	0	4.599476	-2.778665	1.742218
55	6	0	5.120748	-0.799936	0.969112
56	1	0	5.152862	-0.308311	-0.002500
57	1	0	6.131566	-0.844682	1.381031
58	6	0	4.291111	-0.397414	3.310439

59	1	0	3.935258	-1.424785	3.346954
60	1	0	5.307049	-0.335649	3.702089
61	1	0	3.621075	0.240546	3.886007
62	6	0	-2.619461	-0.211023	2.442975
63	16	0	-0.107824	2.142952	-0.068474
64	16	0	0.097569	-2.161957	-0.196168

CO_2 (gas)

E(RB3LYP) = -188.590392621 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	8	0	0.000000	0.000000	1.169356
3	8	0	0.000000	0.000000	-1.169356

CO_2 (DMSO)

E(RB3LYP) = -188.593247772 A.U.

Number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	8	0	0.000000	0.000000	1.169137
3	8	0	0.000000	0.000000	-1.169137