

**Table S1:** M05-2X+D3/6-311++G (d,p) calculated total energies (E, in Hartree) and optimized geometrical parameters in Cartesian coordinates of Triazole.

(1A)				(2A)			
E= -242.259244808				E= -242.289409676			
c	-1.069341	0.420654	0.000013	c	1.116069	0.022761	0.000018
c	0.102392	1.129981	0.000025	c	-0.864868	0.684941	-0.000039
n	0.509067	-1.050010	-0.000022	n	-0.838001	-0.658415	0.000029
h	-2.084371	0.773062	0.000026	h	-1.601421	-1.311354	0.000112
h	0.328209	2.179829	0.000051	h	2.192135	0.029682	-0.000020
h	2.048868	0.260990	-0.000011	h	-1.773817	1.262121	-0.000073
n	1.048499	0.166928	-0.000007	n	0.429982	-1.098650	-0.000041
n	-0.770569	-0.905160	-0.000013	n	0.361719	1.153256	0.000027
(1B)				(2B)			
E= -242.267498278				E= -242.277965735			
c	-0.904897	-0.702356	0.000090	c	-1.077601	0.247455	-0.000007
c	-0.906651	0.700619	-0.000032	c	1.076262	0.252098	0.000028
n	1.044268	0.001360	0.000060	n	-0.681654	-0.990631	0.000028
h	2.049138	0.002283	0.000085	h	-2.099495	0.583631	-0.000009
h	-1.721919	-1.400921	0.000090	h	-0.004268	2.088487	-0.000025
h	-1.724885	1.397735	-0.000096	h	2.097221	0.590900	0.000034
n	0.352884	1.117479	-0.000011	n	0.685870	-0.988040	-0.000038
n	0.355270	-1.117221	-0.000110	n	-0.002134	1.084337	-0.000008

**Table S2a:** M05-2X+D3/6-311++G (d,p) calculated total energies (E, in Hartree) and optimized geometrical parameters in Cartesian coordinates of Triazole-CO<sub>2</sub>.

(1A-CO <sub>2</sub> ) <sub>a</sub>				(1A-CO <sub>2</sub> ) <sub>b</sub>			
E= -430.885972693				E= -430.884583762			
c	-2.541644	-0.501962	0.000016	c	-0.955437	0.985253	0.000047
c	-2.214077	0.829391	0.000009	c	-2.309499	0.781360	0.000000
n	-0.389445	-0.420364	-0.000043	n	-1.235017	-1.158220	-0.000019
h	-3.507684	-0.971651	0.000036	h	-0.390069	1.899141	0.000060
h	-2.797170	1.731288	0.000025	h	-3.154378	1.444230	0.000000
h	-0.213169	1.588387	0.000008	h	-3.254701	-1.130756	0.000154
n	-0.866090	0.821218	0.000004	n	-2.423532	-0.564850	0.000083
n	-1.393996	-1.226971	-0.000005	n	-0.343843	-0.228161	-0.000063
o	2.065189	1.161636	-0.000008	o	2.252249	1.172361	0.000079
c	2.419914	0.057159	0.000002	c	2.450764	0.032294	0.000176
o	2.819759	-1.020727	0.000018	o	2.710368	-1.090790	-0.000274
(1A-CO <sub>2</sub> ) <sub>c</sub>				(1A-CO <sub>2</sub> ) <sub>d</sub>			
E= -430.883326997				E= -430.883161314			
c	-1.636519	1.143716	-0.049681	c	1.538426	-0.619174	-0.931533
c	-2.616985	0.187785	-0.010603	c	2.117420	0.484367	-0.362557
n	-0.613203	-0.754037	0.038692	n	0.592087	-0.377532	0.992473
h	-1.720860	2.213567	-0.097942	h	1.723418	-1.077596	-1.885319
h	-3.689847	0.232315	-0.016783	h	2.878772	1.167682	-0.688554
h	-2.266677	-1.913856	0.084784	h	1.615784	1.271863	1.553268
n	-1.923924	-0.969659	0.043616	n	1.493199	0.585014	0.829221
n	-0.430971	0.519784	-0.017326	n	0.612910	-1.111126	-0.068242
o	2.468972	0.065003	1.149346	o	-2.740915	-0.628261	0.259920
c	2.435604	-0.001064	-0.002936	c	-2.128406	0.255161	-0.155576
o	2.451211	-0.075911	-1.155047	o	-1.542833	1.158441	-0.579366
(1A-CO <sub>2</sub> ) <sub>e</sub>				(1A-CO <sub>2</sub> ) <sub>f</sub>			
E= -430.882688388				E= -430.881911963			
c	-0.909233	-1.103047	0.526959	c	-2.662540	0.922832	-0.016234
c	-1.569809	-0.015240	1.034689	c	-1.292725	0.909475	0.018205
n	-1.229182	0.229238	-1.141145	n	-2.090197	-1.156730	-0.007386
h	-0.566245	-1.993618	1.020990	h	-3.341867	1.755096	-0.030969
h	-1.910116	0.247472	2.018580	h	-0.545520	1.680100	0.039873
h	-2.169427	1.684394	-0.102653	h	-0.087134	-0.840683	0.043653
n	-1.744022	0.775340	-0.044562	n	-0.993733	-0.406069	0.022078
n	-0.722194	-0.906893	-0.805873	n	-3.104629	-0.361890	-0.030879
o	1.516153	1.287358	0.187832	o	4.378227	0.063951	-0.049450
c	2.056978	0.273195	0.068013	c	3.231238	-0.006687	0.002022
o	2.614592	-0.731294	-0.034560	o	2.076597	-0.073378	0.054048
(1A-CO <sub>2</sub> ) <sub>g</sub>				(2A-CO <sub>2</sub> ) <sub>a</sub>			
g to e				E= -430.916180089			
				c	1.456591	1.162150	-0.000477
				c	2.203182	-0.788840	0.001162
				n	0.862127	-0.824604	-0.001755
				h	0.230973	-1.609020	-0.002585
				h	1.413522	2.237399	-0.000591
				h	2.821189	-1.670554	0.002357
				n	0.368027	0.423416	-0.002760
				n	2.616972	0.458839	0.002006
				o	-2.785137	1.023043	0.000846
				c	-2.407106	-0.063678	0.000514
				o	-2.078809	-1.175440	0.000552

(2A-CO <sub>2</sub> ) <sub>b</sub>				(2A-CO <sub>2</sub> ) <sub>c</sub>			
E= -430.915253836				E= -430.912756474			
c	1.383208	1.144300	0.000415	c	-0.809134	-1.182821	-0.123466
c	0.904422	-0.894296	0.000826	c	-1.425877	0.565555	0.841820
n	2.237388	-0.741556	-0.000718	n	-1.681173	0.661889	-0.472047
h	2.957736	-1.441890	-0.001703	h	-2.074661	1.428340	-0.988834
h	1.275116	2.214872	0.000628	h	-0.403891	-2.166187	-0.289470
h	0.402965	-1.847105	0.001342	h	-1.647606	1.344962	1.550382
n	2.560584	0.561880	-0.001101	n	-1.285836	-0.451625	-1.107516
n	0.328278	0.287132	0.001754	n	-0.870274	-0.596420	1.101748
o	-2.225628	-1.183540	-0.000323	o	1.526525	1.304942	-0.142489
c	-2.443339	-0.046901	-0.000490	c	2.012905	0.260567	-0.053937
o	-2.722536	1.071454	-0.000217	o	2.513447	-0.775420	0.028254
(2A-CO <sub>2</sub> ) <sub>d</sub>				(1B-CO <sub>2</sub> ) <sub>a</sub>			
E= -430.912024051				E= -430.893617762			
c	3.061110	-0.252747	-0.004528	c	-1.466649	1.182979	-0.000518
c	1.316112	0.894434	0.002700	c	-2.589812	0.343493	0.000823
n	0.997310	-0.409411	0.003549	n	-0.862357	-0.803703	-0.000542
h	0.085725	-0.832070	0.006870	h	-0.250000	-1.603485	-0.000931
h	4.103057	-0.522512	-0.008785	h	-1.394301	2.255520	-0.000896
h	0.583622	1.683143	0.005975	h	-3.638292	0.580866	0.001796
n	2.108895	-1.159917	-0.001045	n	-2.168318	-0.915487	0.000757
n	2.622817	1.033335	-0.002419	n	-0.381417	0.419019	-0.001376
o	-4.383490	0.065422	-0.007810	o	2.090822	-1.162713	-0.000138
c	-3.236258	-0.019889	0.000259	c	2.416350	-0.050820	0.000263
o	-2.081678	-0.103846	0.008405	o	2.785167	1.039510	0.000733
(1B-CO <sub>2</sub> ) <sub>b</sub>				(1B-CO <sub>2</sub> ) <sub>c</sub>			
E= -430.893603184				E= -430.887707097			
c	-2.592032	0.334456	0.038085	c	1.112242	0.701008	0.040573
c	-1.477545	1.183467	-0.013668	c	1.115578	-0.702268	0.039215
n	-0.855958	-0.797575	-0.032302	n	3.062428	0.004162	-0.048580
h	-0.237460	-1.592438	-0.050232	h	4.066331	0.006631	-0.096455
h	-3.641432	0.562937	0.083044	h	0.290576	1.392420	0.078836
h	-1.415069	2.256618	-0.021222	h	0.297179	-1.397598	0.076032
n	-0.386061	0.429493	-0.057880	n	2.374974	-1.115056	-0.018499
n	-2.159677	-0.920719	0.025092	n	2.369629	1.120030	-0.016230
o	2.085167	-1.161761	0.007258	o	-2.151611	-0.019810	0.083924
c	2.417451	-0.051752	0.012800	c	-3.304199	-0.002400	0.001906
o	2.792157	1.036444	0.020334	o	-4.454019	0.014379	-0.079601
(2B-CO <sub>2</sub> ) <sub>a</sub>				(2B-CO <sub>2</sub> ) <sub>b</sub>			
E= -430.904074799				E= -430.903146414			
c	2.461056	-0.585383	0.000096	c	1.712323	-1.077933	-0.000870
c	0.894750	0.895654	0.000023	c	1.712886	1.077824	0.000248
n	1.326266	-1.218440	0.000058	n	0.474510	-0.683658	-0.009124
h	3.435967	-1.039496	0.000116	h	2.049852	-2.099245	0.000745
h	2.937051	1.492267	0.000005	h	3.549645	-0.000541	0.010522
h	0.374724	1.837352	-0.000068	h	2.050787	2.099000	0.003147
n	0.333797	-0.278632	0.000130	n	0.474880	0.684123	-0.007888
n	2.248526	0.761230	0.000038	n	2.545373	-0.000281	0.003996
o	-2.740565	-1.075055	0.000018	o	-2.408948	0.000763	-1.150619
c	-2.441720	0.037344	-0.000122	c	-2.373682	0.000610	0.003483
o	-2.208482	1.171940	-0.000219	o	-2.393901	-0.001202	1.158060
(2B-CO <sub>2</sub> ) <sub>c</sub>				(2B-CO <sub>2</sub> ) <sub>d</sub>			
E= -430.902754480				E= -430.900807003			

c	-1.453825	-0.066943	-1.075949	c	-1.803525	1.075838	0.008823
c	-1.454945	0.042740	1.074984	c	-1.805608	-1.074867	0.008139
n	-0.597745	-0.941532	-0.638193	n	-3.043397	0.685501	-0.037773
h	-1.683427	0.128147	-2.108596	h	-1.464488	2.096684	0.022122
h	-2.715857	1.321245	-0.069169	h	0.034826	-0.001423	0.076020
h	-1.685109	0.343374	2.081755	h	-1.468518	-2.096373	0.020802
n	-0.598407	-0.872108	0.729182	n	-3.044715	-0.682064	-0.038214
n	-2.031377	0.587315	-0.031308	n	-0.970387	-0.000341	0.039623
o	1.485191	1.294602	-0.052355	o	4.512816	0.006514	-0.064558
c	2.085274	0.305663	-0.013372	c	3.364874	-0.001162	0.001312
o	2.717069	-0.656758	0.022889	o	2.208837	-0.008941	0.067803
(2B-CO <sub>2</sub> ) <sub>e</sub>							
E= -430.898544575							
c	1.061849	-0.179882	-0.000021				
c	3.077269	0.583384	0.000135				
n	1.869326	-1.199019	-0.000111				
h	-0.012785	-0.220521	-0.000062				
h	1.415771	1.919559	0.000096				
h	3.912632	1.261142	0.000240				
n	3.149048	-0.714457	-0.000012				
n	1.774225	0.981739	0.000056				
o	-2.428245	0.392211	0.000051				
c	-3.532916	0.050088	-0.000023				
o	-4.634382	-0.287157	-0.000095				

**Table S2b:** Harmonic frequencies and IR of the Triazole-CO<sub>2</sub> complexes computed at the M05-2X+D3/6-311+G(d,p) level.

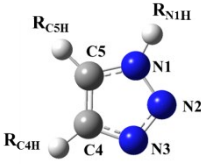
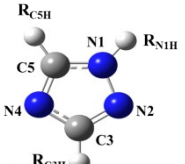
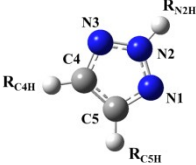
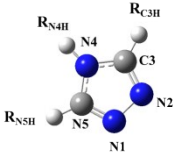
Molecular species	Frequencies	IR	Molecular species	Frequencies	IR
(1A-CO <sub>2</sub> ) <sub>a</sub>	37.9814	7.8118	(2A-CO <sub>2</sub> ) <sub>a</sub>	38.1047	0.2693
	62.6138	0.3553		62.4896	2.4420
	64.2096	7.5704		69.3202	6.1136
	113.4499	5.2447		106.9516	1.4814
	162.3429	1.0447		165.9852	1.0460
	635.6490	13.1172		627.3758	53.2229
	677.1198	94.1570		678.5710	98.8680
	694.3538	0.1032		698.2629	19.7396
	703.0114	89.8412		706.1722	3.7576
	756.2975	32.0283		721.6166	92.2631
	806.4077	58.4856		893.0595	15.7331
	891.1492	5.1777		934.1144	11.4248
	979.5382	2.3872		989.0508	4.9271
	1003.7512	1.9368		1014.5790	25.9684
	1092.9133	34.9308		1119.5871	55.9373
	1134.4823	47.6343		1175.8880	39.3175
	1172.6124	12.8762		1219.1735	2.7222
	1221.8631	14.7100		1302.2971	4.7982
	1368.1035	22.3835		1362.4303	24.0103
	1412.0356	2.1756		1413.6145	1.3646
1415.9092	7.5940	1433.3835	20.9106		
1505.5733	0.3181	1518.7272	41.7329		
1586.2035	15.1555	1601.1424	33.7585		
2459.9837	753.3587	2462.2280	747.4088		
3316.4365	1.3943	3306.7814	0.4341		
3344.9336	1.6032	3316.4599	1.6326		
3697.9981	154.970	3700.0188	151.8628		

(1A-CO <sub>2</sub> ) <sub>b</sub>	12.4617	13.8575	(2A-CO <sub>2</sub> ) <sub>b</sub>	46.6328	2.0142
	39.9748	0.0029		54.2090	1.5865
	41.1196	7.3697		54.4829	5.0208
	90.1389	0.3406		90.4755	0.0324
	150.3672	0.6481		159.3763	1.0735
	620.8026	45.2820		612.1157	74.7718
	670.6456	102.0378		669.0969	104.8795
	671.6635	39.4982		697.2207	13.0066
	702.4911	46.3313		703.8698	16.6476
	748.2623	8.2870		715.0118	72.5828
	803.9606	58.1222		897.5431	14.6549
	899.6498	7.4811		934.4631	11.7122
	978.0866	2.3356		991.7094	7.7578
	1003.5276	0.6987		1014.7317	15.0616
	1091.6679	29.3170		1117.2008	59.4256
	1131.5842	48.2051		1173.7401	23.5483
	1172.7561	3.0773		1215.3503	9.2721
	1215.2653	8.6480		1303.6997	1.8424
	1364.6988	24.5941		1365.3919	22.5872
	1412.2763	1.5753		1413.3743	1.4480
1415.0018	1.3707	1445.7381	11.7381		
1496.7597	0.0743	1517.7169	25.6602		
1589.0008	7.4134	1611.0432	30.7396		
2457.5475	738.1278	2460.2636	732.8430		
3327.8409	3.6065	3291.5292	3.2283		
3346.3942	1.5361	3311.5767	1.2405		
3720.5998	123.9707	3727.2754	120.0834		
(1A-CO <sub>2</sub> ) <sub>c</sub>	21.0596	9.7938	(2A-CO <sub>2</sub> ) <sub>c</sub>	27.3133	0.7913
	41.7786	3.2624		50.5967	1.9466
	47.2917	6.3721		63.0392	3.2720
	81.9093	0.8136		72.7096	4.5295
	113.6989	1.0416		98.5581	0.2546
	616.0736	47.1979		604.6762	86.4051
	670.7545	43.4211		688.2103	61.0194
	684.7991	84.1788		693.7168	23.7259
	701.0913	37.2298		696.9645	23.9561
	748.2421	7.8438		714.2929	52.0242
	802.7326	62.1284		888.8904	14.4564
	887.8179	3.6539		927.0868	13.1381
	979.6148	1.4797		986.4027	4.4204
	1002.2775	1.0140		1015.2192	12.9475
	1095.0912	27.4619		1119.3485	47.8394
	1129.8237	38.2029		1172.7772	22.4422
	1174.9768	4.5358		1215.0063	6.3812
	1219.2716	6.9062		1304.8502	0.9221
	1366.3172	22.1549		1358.4336	23.3770
	1414.4235	1.0105		1417.4739	0.1451
1417.4621	3.0002	1442.4678	14.6337		
1502.7761	0.1511	1516.7992	22.4791		
1592.3526	6.5436	1606.6777	28.0538		
2460.2368	758.5596	2465.9410	684.0128		
3317.4803	2.5606	3299.2316	0.8658		
3342.0572	2.1289	3305.7965	1.0780		
3727.5503	122.8058	3728.2943	119.3973		
(1A-CO <sub>2</sub> ) <sub>d</sub>	7.3889	6.7639	(2A-CO <sub>2</sub> ) <sub>d</sub>	1.1032	1.9080
	34.1110	5.0939		13.5608	2.3183
	44.1236	5.5234		44.9583	0.0062
	67.0047	4.2543		60.2127	3.3535
	103.9214	2.5492		81.8601	1.4097
	618.4463	50.5994		627.0157	53.6250
	667.8041	47.4178		693.1649	41.6509
	684.8564	66.8296		696.7265	42.0371
	693.0470	35.4691		703.2568	0.9604
	747.9555	9.5217		726.2477	76.8762
	801.9810	58.6266		876.9830	14.3060
	887.3966	4.6192		923.7313	12.0277
	977.4661	1.9282		986.8128	9.4383
	1003.3635	0.9871		1016.8870	11.6762
	1095.8885	26.7816		1118.0726	52.5559
	1133.4718	36.7771		1170.6574	42.3225
	1174.3398	5.7105		1218.0488	4.5933
	1219.6099	6.2627		1301.9632	2.9063
	1361.0756	22.2506		1363.2104	25.9193
	1413.4227	0.4930		1418.5684	2.0113
1419.3939	1.5396	1440.4216	19.1236		
1501.0267	0.2603	1514.4267	25.3697		
1590.4983	6.6278	1606.4165	44.7949		
2459.4742	743.1264	2467.7826	1042.1548		
3318.7337	2.3123	3287.5693	1.6619		
3339.2891	1.5363	3301.9682	1.4768		
3722.6046	120.591	3735.2311	209.8484		
(1A-CO <sub>2</sub> ) <sub>e</sub>	31.2772	2.9463	(2B-CO <sub>2</sub> ) <sub>a</sub>	47.6950	17.6638
	52.9624	15.8376		59.4867	0.3886
	62.1129	0.0453		60.6265	11.5249
	86.7977	3.2307		96.0058	2.0705
	118.7334	0.4944		160.4976	1.7488

	628.4333 674.7569 684.7617 697.7932 749.3838 805.7146 886.2947 976.8096 1003.6140 1093.5254 1131.0402 1172.2756 1213.7668 1360.9247 1414.4586 1415.0922 1499.5528 1589.6058 2459.1828 3313.6173 3341.5929 3720.5176	38.2752 64.3198 57.4339 37.1714 11.8933 61.6210 5.1136 1.5418 0.7086 25.4285 33.2218 4.1268 7.4055 19.2725 0.3840 2.1631 0.1626 7.2794 699.9803 2.4120 2.6638 122.9823		572.3703 669.5352 677.3740 702.9204 711.4324 836.5520 876.1566 971.9916 998.2404 1093.3318 1117.8050 1145.3154 1255.7677 1356.7867 1414.0401 1454.2880 1573.3648 1574.3691 2461.9949 3302.2578 3314.6272 3737.9030	126.6048 103.6872 2.3438 36.6815 3.5195 1.5788 31.7295 0.1314 2.6533 29.2848 5.2461 34.7841 1.4111 0.9159 1.9606 34.4259 27.8345 17.1696 738.2081 0.9095 2.1428 109.0847
(1A-CO <sub>2</sub> ) <sub>f</sub>	6.1624 14.5166 41.3577 57.9856 79.4358 633.4822 688.0303 693.9268 696.1923 758.3670 793.9298 881.2997 977.5966 1000.0495 1090.7612 1132.5970 1174.5656 1216.7076 1361.2030 1417.4487 1420.3596 1497.6158 1588.7952 2470.9122 3317.7382 3336.1508 3724.4746	4.4773 6.0026 0.3700 5.3003 1.0871 17.6040 27.6077 69.0774 44.5264 22.6742 57.4207 6.6335 0.7240 1.7834 30.2759 49.4431 10.4854 13.6841 24.7775 5.3992 5.8313 2.2400 10.7592 1048.8468 2.5132 0.1691 212.5526	(2B-CO <sub>2</sub> ) <sub>b</sub>	6.5016 53.6682 60.3533 99.8229 122.7561 544.7403 668.0670 693.2003 697.0381 708.6425 828.3329 864.3838 967.8805 998.4215 1083.1214 1116.6417 1141.7728 1253.8058 1357.4647 1412.4225 1454.7159 1577.2727 1577.6842 2455.9595 3312.4687 3316.5894 3742.2873	22.0712 12.3715 0.0286 0.1583 1.0485 127.4168 0.0022 87.8046 36.4760 0.0005 0.0001 33.6610 0.0203 4.1322 17.4274 5.5975 32.7807 0.4204 1.2082 1.0185 32.7800 15.5433 40.5132 754.6329 1.5780 0.0681 113.3567
(1A-CO <sub>2</sub> ) <sub>g</sub>	g to e	g to e	(2B-CO <sub>2</sub> ) <sub>c</sub>	28.2486 47.1072 58.9871 77.6844 95.7568 558.8680 671.6656 687.4753 697.1302 706.9777 832.4433 868.1480 967.6572 996.0869 1078.4415 1117.8786 1141.8917 1252.9890 1356.0931 1415.0652 1452.0551 1570.8693 1574.3431 2462.5611 3309.6496 3315.1557 3735.7300	23.0779 6.3323 0.2363 6.4794 2.5081 131.2443 0.5994 70.2589 31.1826 3.5232 0.0254 31.5183 0.0179 3.4603 17.3669 5.6117 30.0688 0.4418 1.4280 0.6861 30.8737 26.6290 26.9603 739.2098 1.9144 0.2712 111.3001
(1B-CO <sub>2</sub> ) <sub>a</sub>	33.2452 58.9089 66.4632 105.6963 162.9113 651.9066 680.3186 690.0328 699.9116 758.7124	0.0015 0.1181 0.9291 0.2226 0.1251 20.2788 95.3679 0.2912 33.9294 69.1316	(2B-CO <sub>2</sub> ) <sub>d</sub>	24.3687 26.0098 44.7452 63.4791 73.2388 596.1314 690.6494 693.1785 695.2342 708.9071	4.0262 10.5810 8.2327 12.4800 1.0247 111.6824 0.2724 43.0862 56.2365 0.0000

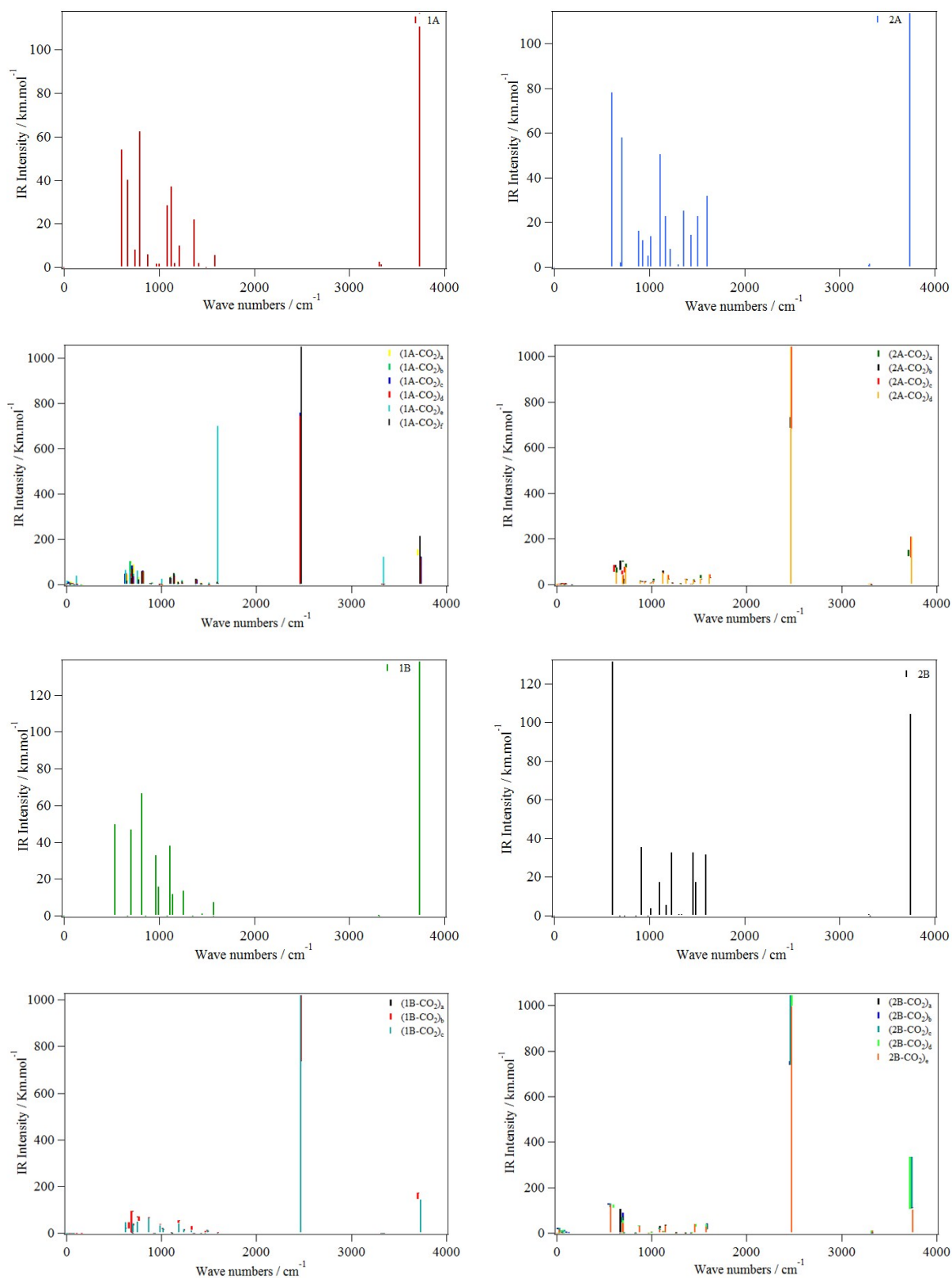
	865.0283 920.5892 987.7378 1013.8852 1100.8670 1174.1303 1237.1652 1312.2994 1337.5919 1414.8244 1462.9961 1480.2995 1591.5085 2464.1850 3310.0706 3325.9284 3700.2525	67.7014 0.4685 37.8964 16.8663 0.2925 52.3186 12.3853 30.4007 0.4370 1.1779 7.4525 7.5471 3.2018 738.3308 0.4427 0.0362 170.2010		824.1441 861.3055 970.1915 997.7235 1084.0093 1129.8656 1144.1122 1252.4585 1353.8368 1419.4011 1460.4817 1572.9628 1573.8603 2469.4526 3310.0530 3314.2680 3717.0882	0.0001 34.1071 0.0640 0.3487 23.1587 3.5249 33.3766 0.7651 1.7917 3.3387 28.7326 13.8431 39.0991 1045.1075 0.4186 0.1935 335.6848
(1B-CO <sub>2</sub> ) <sub>b</sub>	30.7077 58.9399 64.6968 106.3419 161.2778 653.6178 679.8444 689.6865 699.6788 759.7491 865.1444 920.6186 987.9218 1014.3924 1102.2687 1175.1521 1236.8930 1312.8461 1338.5295 1414.2852 1463.5280 1482.4967 1592.5254 2463.1338 3310.9891 3326.3871 3697.5122	0.0026 0.1884 0.9373 0.2188 0.1127 19.3761 94.6301 0.2731 34.1675 69.6421 68.0498 0.4248 37.9841 16.8101 0.3326 53.1314 12.1592 30.1858 0.4858 1.1720 7.9250 7.5901 3.3635 739.3653 0.4454 0.0209 171.6169	(2B-CO <sub>2</sub> ) <sub>e</sub>	22.0453 24.6481 34.5812 45.8813 60.9854 565.6558 677.3225 697.4252 698.2031 707.9885 830.1870 874.6757 967.8689 996.5596 1083.7533 1114.1871 1141.4112 1255.5539 1353.3225 1420.1898 1452.1545 1570.4270 1573.9166 2471.4606 3316.0489 3322.8758 3746.9035	0.2207 12.5559 0.2188 4.6088 0.3079 125.0713 1.2614 44.3287 42.3753 0.0534 3.2157 31.0881 0.0479 5.2959 16.3443 6.9398 33.8160 0.2088 1.7979 0.8100 39.4141 28.2887 24.9502 995.6522 3.0653 10.2809 101.7656
(1B-CO <sub>2</sub> ) <sub>c</sub>	12.8947 21.6454 48.1285 66.0821 72.4095 620.5925 692.0132 696.2274 697.6462 746.1587 868.3897 923.0905 986.3429 1017.0040 1111.2136 1183.2563 1233.3641 1315.6054 1342.6446 1417.2756 1464.1168 1488.3815 1594.6944 2463.6377 3321.2101 3335.7719 3731.4156	0.0121 0.0054 0.0042 0.0409 0.0027 44.9131 0.0350 40.3803 40.6720 49.7141 65.0828 0.0007 31.6035 21.0914 2.9616 41.4310 16.8776 11.3995 0.6185 0.1989 1.1145 13.9217 0.1942 1019.5104 0.1121 0.0100 143.9539			

**Table S3:** Comparison of some internal distances of isolated CO<sub>2</sub>, triazoles and TZ-CO<sub>2</sub> complexes.

Definition of the parameters	Complexes	Distance	M052X+D3/6-311++G(d,p)
	CO <sub>2</sub>	R <sub>CO</sub>	1.154
 <p><b>1H-1,2,3-triazole: 1A</b></p>	1A	R <sub>N1H</sub> R <sub>C4H</sub> R <sub>C5H</sub>	1.004 1.073 1.073
	(1A-CO <sub>2</sub> ) <sub>a</sub>	R <sub>N1H</sub> R <sub>CO</sub>	1.007 1.160
	(1A-CO <sub>2</sub> ) <sub>c</sub>	R <sub>C4H</sub> R <sub>CO</sub>	1.074 1.157
	(1A-CO <sub>2</sub> ) <sub>f</sub>	R <sub>N1H</sub> R <sub>CO</sub>	1.005 1.157
 <p><b>1H-1,2,4-triazole: 2A</b></p>	2A	R <sub>N1H</sub> R <sub>C3H</sub> R <sub>C5H</sub>	1.004 1.076 1.076
	(2A-CO <sub>2</sub> ) <sub>a</sub>	R <sub>N1H</sub> R <sub>CO</sub>	1.006 1.159
	(2A-CO <sub>2</sub> ) <sub>b</sub>	R <sub>C5H</sub> R <sub>CO</sub>	1.076 1.157
	(2A-CO <sub>2</sub> ) <sub>d</sub>	R <sub>N1H</sub> R <sub>CO</sub>	1.004 1.157
 <p><b>2H-1,2,3-triazole: 1B</b></p>	1B	R <sub>N2H</sub> R <sub>C4H</sub> R <sub>C5H</sub>	1.004 1.074 1.074
	(1B-CO <sub>2</sub> ) <sub>a</sub>	R <sub>N2H</sub> R <sub>CO</sub>	1.007 1.158
	(1B-CO <sub>2</sub> ) <sub>c</sub>	R <sub>C4H</sub> R <sub>CO</sub>	1.074 1.155
 <p><b>4H-1,2,4-triazole: 2B</b></p>	2B	R <sub>N4H</sub> R <sub>C3H</sub> R <sub>C5H</sub>	1.004 1.075 1.075
	(2B-CO <sub>2</sub> ) <sub>a</sub>	R <sub>C3H</sub> R <sub>CO</sub>	1.075 1.158
	(2B-CO <sub>2</sub> ) <sub>d</sub>	R <sub>N4H</sub> R <sub>CO</sub>	1.005 1.158
	(2B-CO <sub>2</sub> ) <sub>e</sub>	R <sub>C3H</sub> R <sub>CO</sub>	1.075 1.156



**Figure S1:** Simulated IR spectra of TZ (1A, 2A, 1B, 2B) and of TZ-CO<sub>2</sub>.





















288.643	5.41433	288.643	1.32142	288.643	-0.824975	288.643	-2.01477	288.643	-2.27609	288.643	-2.25003	288.643	-1.48923	288.643	-0.512658
290.427	6.23336	290.427	1.87771	290.427	-0.440013	290.427	-1.7512	290.427	-2.07837	290.427	-2.1224	290.427	-1.43239	290.427	-0.493997
292.211	7.05648	292.211	2.44129	292.211	-0.0461173	292.211	-1.47535	292.211	-1.87482	292.211	-1.98599	292.211	-1.36996	292.211	-0.473254
293.995	7.86655	293.995	3.0012	293.995	0.349655	293.995	-1.19199	293.995	-1.66772	293.995	-1.84261	293.995	-1.30254	293.995	-0.450557
295.779	8.64643	295.779	3.54653	295.779	0.740245	295.779	-0.905915	295.779	-1.45938	295.779	-1.69408	295.779	-1.23072	295.779	-0.426034
297.563	9.37901	297.563	4.06632	297.563	1.11859	297.563	-0.621901	297.563	-1.25209	297.563	-1.54221	297.563	-1.15509	297.563	-0.399812
299.347	10.0471	299.347	4.54966	299.347	1.47764	299.347	-0.344733	299.347	-1.04816	299.347	-1.38881	299.347	-1.07625	299.347	-0.372021
301.131	10.6337	301.131	4.9856	301.131	1.81033	301.131	-0.0791908	301.131	-0.849884	301.131	-1.2357	301.131	-0.994776	301.131	-0.342788
302.915	11.1216	302.915	5.3632	302.915	2.1096	302.915	0.169943	302.915	-0.659556	302.915	-1.08469	302.915	-0.911272	302.915	-0.312241
304.698	11.4936	304.698	5.67154	304.698	2.36839	304.698	0.397885	304.698	-0.479475	304.698	-0.937605	304.698	-0.826328	304.698	-0.280509
306.482	11.7363	306.482	5.90196	306.482	2.58105	306.482	0.600674	306.482	-0.311542	306.482	-0.795992	306.482	-0.740492	306.482	-0.247722
308.266	11.8613	308.266	6.06115	308.266	2.75133	308.266	0.77983	308.266	-0.154975	308.266	-0.659714	308.266	-0.654017	308.266	-0.21404
310.05	11.8902	310.05	6.16209	310.05	2.88681	310.05	0.939126	310.05	-0.00789614	310.05	-0.527925	310.05	-0.567038	310.05	-0.179634
311.834	11.8448	311.834	6.21776	311.834	2.99513	311.834	1.08234	311.834	0.131579	311.834	-0.399781	311.834	-0.479686	311.834	-0.144673
313.618	11.7468	313.618	6.24118	313.618	3.08389	313.618	1.21326	313.618	0.265332	313.618	-0.274437	313.618	-0.392096	313.618	-0.109326
315.402	11.6179	315.402	6.24534	315.402	3.1607	315.402	1.33565	315.402	0.395247	315.402	-0.151047	315.402	-0.3044	315.402	-0.0737647
317.186	11.4798	317.186	6.24324	317.186	3.23319	317.186	1.45331	317.186	0.523207	317.186	-0.0287645	317.186	-0.216731	317.186	-0.0381583
318.97	11.3544	318.97	6.24787	318.97	3.30897	318.97	1.57	318.97	0.651094	318.97	0.0932545	318.97	-0.129222	318.97	-0.0026769
320.754	11.2633	320.754	6.27223	320.754	3.39564	320.754	1.68952	320.754	0.780792	320.754	0.215856	320.754	-0.0420065	320.754	0.0325095
322.538	11.2283	322.538	6.32932	322.538	3.50084	322.538	1.81563	322.538	0.914184	322.538	0.339885	322.538	0.0447835	322.538	0.067231
324.322	11.2711	324.322	6.43214	324.322	3.63217	324.322	1.95212	324.322	1.05315	324.322	0.466187	324.322	0.131015	324.322	0.101318
326.106	11.4123	326.106	6.59299	326.106	3.79679	326.106	2.10255	326.106	1.19943	326.106	0.59551	326.106	0.21652	326.106	0.134594
327.889	11.6576	327.889	6.81452	327.889	3.99568	327.889	2.2674	327.889	1.35276	327.889	0.727244	327.889	0.300668	327.889	0.16681
329.673	12.0014	329.673	7.09234	329.673	4.22528	329.673	2.44487	329.673	1.51139	329.673	0.859787	329.673	0.382486	329.673	0.197663
331.457	12.4381	331.457	7.42188	331.457	4.48192	331.457	2.63316	331.457	1.67354	331.457	0.991514	331.457	0.460992	331.457	0.226846
333.241	12.9619	333.241	7.7986	333.241	4.76194	333.241	2.83043	333.241	1.83745	333.241	1.1208	333.241	0.535207	333.241	0.254056
335.025	13.5672	335.025	8.21793	335.025	5.06167	335.025	3.03485	335.025	2.00133	335.025	1.24602	335.025	0.60415	335.025	0.278986
336.809	14.2481	336.809	8.67532	336.809	5.37745	336.809	3.2446	336.809	2.16342	336.809	1.36556	336.809	0.666841	336.809	0.301332
338.593	14.9992	338.593	9.1662	338.593	5.70561	338.593	3.45785	338.593	2.32194	338.593	1.47778	338.593	0.722299	338.593	0.320788
340.377	15.8145	340.377	9.68603	340.377	6.04249	340.377	3.67276	340.377	2.47512	340.377	1.58106	340.377	0.769543	340.377	0.33705
342.161	16.6884	342.161	10.2302	342.161	6.38442	342.161	3.88752	342.161	2.62117	342.161	1.67378	342.161	0.807594	342.161	0.349811
343.945	17.6152	343.945	10.7943	343.945	6.72774	343.945	4.10029	343.945	2.75833	343.945	1.75431	343.945	0.835471	343.945	0.358768
345.729	18.5892	345.729	11.3736	345.729	7.06884	345.729	4.30928	345.729	2.88486	345.729	1.82107	345.729	0.85222	345.729	0.363624
347.513	19.6049	347.513	11.965	347.513	7.40585	347.513	4.5137	347.513	3.00035	347.513	1.87389	347.513	0.857886	347.513	0.364426
349.296	20.6571	349.296	12.5669	349.296	7.73916	349.296	4.71404	349.296	3.10609	349.296	1.91441	349.296	0.853784	349.296	0.361656
351.08	21.7406	351.08	13.1777	351.08	8.0693	351.08	4.91088	351.08	3.20346	351.08	1.94439	351.08	0.841308	351.08	0.355824
352.864	22.8501	352.864	13.7961	352.864	8.3968	352.864	5.10482	352.864	3.29386	352.864	1.96558	352.864	0.821854	352.864	0.347441
354.648	23.9804	354.648	14.4204	354.648	8.72219	354.648	5.29643	354.648	3.37869	354.648	1.97975	354.648	0.796817	354.648	0.337017
356.432	25.1264	356.432	15.0491	356.432	9.04599	356.432	5.48629	356.432	3.45934	356.432	1.98865	356.432	0.767594	356.432	0.325062
358.216	26.2828	358.216	15.6809	358.216	9.36873	358.216	5.67499	358.216	3.53721	358.216	1.99404	358.216	0.73558	358.216	0.312086
360	27.4444	360	16.3142	360	9.69095	360	5.86311	360	3.61367	360	1.99766	360	0.70217	360	0.2986

## 2A- CO<sub>2</sub>

angle	R <sub>c</sub> - 0.3	angle	R <sub>c</sub> - 0.15	angle	R <sub>c</sub>	angle	R <sub>c</sub> + 0.15	angle	R <sub>c</sub> + 0.3	angle	R <sub>c</sub> + 0.5	angle	R <sub>c</sub> + 1	angle	R <sub>c</sub> + 2
5	31.4996	5	18.0666	5	10.1791	5	5.68705	5	3.04586	5	1.25199	5	0.10118	5	0.0808765









335.025	17.3962	335.025	8.03251	335.025	4.33251	335.025	2.21252	335.025	1.11706	335.025	0.937274	335.025	0.152643	335.025	0.195822
336.809	18.3361	336.809	8.35283	336.809	4.58572	336.809	2.39054	336.809	1.27015	336.809	0.956601	336.809	0.210692	336.809	0.208765
338.593	19.44	338.593	8.80621	338.593	4.91526	338.593	2.61322	338.593	1.44615	338.593	0.983465	338.593	0.266417	338.593	0.220313
340.377	20.6537	340.377	9.37319	340.377	5.30775	340.377	2.87188	340.377	1.63862	340.377	1.0179	340.377	0.318063	340.377	0.230033
342.161	21.9231	342.161	10.0343	342.161	5.74983	342.161	3.15779	342.161	1.84112	342.161	1.05994	342.161	0.363875	342.161	0.237495
343.945	23.194	343.945	10.7702	343.945	6.22814	343.945	3.46227	343.945	2.0472	343.945	1.10963	343.945	0.402101	343.945	0.242264
345.729	24.4128	345.729	11.5614	345.729	6.72943	345.729	3.77669	345.729	2.2505	345.729	1.16697	345.729	0.431019	345.729	0.243919
347.513	25.5531	347.513	12.3948	347.513	7.24535	347.513	4.09588	347.513	2.44771	347.513	1.23161	347.513	0.450164	347.513	0.242388
349.296	26.6227	349.296	13.2646	349.296	7.77371	349.296	4.41898	349.296	2.63937	349.296	1.30265	349.296	0.460669	349.296	0.238043
351.08	27.6319	351.08	14.1657	351.08	8.31275	351.08	4.74545	351.08	2.82627	351.08	1.37918	351.08	0.463768	351.08	0.231286
352.864	28.5906	352.864	15.0927	352.864	8.86067	352.864	5.07471	352.864	3.00921	352.864	1.46029	352.864	0.460695	352.864	0.222519
354.648	29.5089	354.648	16.0406	354.648	9.41571	354.648	5.40622	354.648	3.18897	354.648	1.54506	354.648	0.452684	354.648	0.212145
356.432	30.397	356.432	17.0041	356.432	9.97608	356.432	5.7394	356.432	3.36635	356.432	1.63257	356.432	0.44097	356.432	0.200565
358.216	31.2649	358.216	17.978	358.216	10.54	358.216	6.0737	358.216	3.54215	358.216	1.72191	358.216	0.426787	358.216	0.188181
360	32.1228	360	18.957	360	11.1057	360	6.40857	360	3.71715	360	1.81217	360	0.41137	360	0.175395

## 2B-CO<sub>2</sub>

angle	R <sub>c</sub> - 0.3	angle	R <sub>c</sub> - 0.15	angle	R <sub>c</sub>	angle	R <sub>c</sub> + 0.15	angle	R <sub>c</sub> + 0.3	angle	R <sub>c</sub> + 0.5	angle	R <sub>c</sub> + 1	angle	R <sub>c</sub> + 2
5	35.4215	5	20.911	5	12.1968	5	7.05152	5	4.06799	5	1.98684	5	0.510626	5	0.288949
6.78392	34.1082	6.78392	19.9341	6.78392	11.4801	6.78392	6.52596	6.78392	3.68046	6.78392	1.72492	6.78392	0.403171	6.78392	0.2624
8.56784	32.7947	8.56784	18.9591	8.56784	10.7659	8.56784	6.00281	8.56784	3.29507	8.56784	1.46472	8.56784	0.296537	8.56784	0.236006
10.3518	31.4809	10.3518	17.9877	10.3518	10.0565	10.3518	5.48448	10.3518	2.914	10.3518	1.20794	10.3518	0.191547	10.3518	0.209923
12.1357	30.1667	12.1357	17.0219	12.1357	9.35431	12.1357	4.97338	12.1357	2.53938	12.1357	0.956299	12.1357	0.0890226	12.1357	0.184307
13.9196	28.8517	13.9196	16.0633	13.9196	8.66182	13.9196	4.47193	13.9196	2.17338	13.9196	0.711514	13.9196	-0.0102148	13.9196	0.159311
15.7035	27.536	15.7035	15.1138	15.7035	7.98144	15.7035	3.98252	15.7035	1.81814	15.7035	0.475295	15.7035	-0.105343	15.7035	0.135093
17.4874	26.2193	17.4874	14.1753	17.4874	7.31557	17.4874	3.50757	17.4874	1.47583	17.4874	0.249357	17.4874	-0.195541	17.4874	0.111806
19.2714	24.9015	19.2714	13.2496	19.2714	6.66663	19.2714	3.0495	19.2714	1.14859	19.2714	0.0354118	19.2714	-0.279986	19.2714	0.0896078
21.0553	23.5824	21.0553	12.3384	21.0553	6.03705	21.0553	2.6107	21.0553	0.838584	21.0553	-0.164826	21.0553	-0.357857	21.0553	0.068652
22.8392	22.2618	22.8392	11.4437	22.8392	5.42924	22.8392	2.1936	22.8392	0.547956	22.8392	-0.349644	22.8392	-0.428332	22.8392	0.0490945
24.6231	20.9397	24.6231	10.5673	24.6231	4.84563	24.6231	1.8006	24.6231	0.278863	24.6231	-0.517328	24.6231	-0.490589	24.6231	0.0310908
26.407	19.6183	26.407	9.71229	26.407	4.2893	26.407	1.43439	26.407	0.0335436	26.407	-0.666204	26.407	-0.543879	26.407	0.0147847
28.191	18.3202	28.191	8.89214	28.191	3.76847	28.191	1.09988	28.191	-0.185124	28.191	-0.794892	28.191	-0.588015	28.191	0.000233673
29.9749	17.077	29.9749	8.12505	29.9749	3.29371	29.9749	0.802982	29.9749	-0.373965	29.9749	-0.902149	29.9749	-0.623068	29.9749	-0.0125452
31.7588	15.9204	31.7588	7.42927	31.7588	2.87564	31.7588	0.549606	31.7588	-0.5298	31.7588	-0.986732	31.7588	-0.64911	31.7588	-0.023535
33.5427	14.8821	33.5427	6.82299	33.5427	2.52484	33.5427	0.345673	33.5427	-0.649451	33.5427	-1.0474	33.5427	-0.666214	33.5427	-0.0327188
35.3266	13.9938	35.3266	6.32447	35.3266	2.25191	35.3266	0.197103	35.3266	-0.729743	35.3266	-1.08291	35.3266	-0.674452	35.3266	-0.0400796
37.1106	13.2872	37.1106	5.95191	37.1106	2.06746	37.1106	0.109815	37.1106	-0.767496	37.1106	-1.09202	37.1106	-0.673898	37.1106	-0.0456005
38.8945	12.794	38.8945	5.72354	38.8945	1.98207	38.8945	0.0897261	38.8945	-0.759533	38.8945	-1.07348	38.8945	-0.664625	38.8945	-0.0492647
40.6784	12.5459	40.6784	5.6576	40.6784	2.00635	40.6784	0.142756	40.6784	-0.702678	40.6784	-1.02606	40.6784	-0.646704	40.6784	-0.0510551
42.4623	12.5746	42.4623	5.7723	42.4623	2.15089	42.4623	0.274823	42.4623	-0.593751	42.4623	-0.948515	42.4623	-0.620209	42.4623	-0.0509549
44.2462	12.9118	44.2462	6.08587	44.2462	2.42629	44.2462	0.491845	44.2462	-0.429575	44.2462	-0.839597	44.2462	-0.585211	44.2462	-0.048947
46.0302	13.5869	46.0302	6.61509	46.0302	2.8422	46.0302	0.799133	46.0302	-0.207365	46.0302	-0.698286	46.0302	-0.541841	46.0302	-0.0450335
47.8141	14.5922	47.8141	7.35295	47.8141	3.3928	47.8141	1.19203	47.8141	0.0692498	47.8141	-0.52713	47.8141	-0.491142	47.8141	-0.0395235
49.598	15.8895	49.598	8.27304	49.598	4.05957	49.598	1.65772	49.598	0.391402	49.598	-0.3316	49.598	-0.434908	49.598	-0.0329775
51.3819	17.4398	51.3819	9.34837	51.3819	4.82368	51.3819	2.18317	51.3819	0.750067	51.3819	-0.117252	51.3819	-0.374954	51.3819	-0.0259633









299.347	27.8436	299.347	16.2026	299.347	9.46289	299.347	5.23101	299.347	2.74269	299.347	1.00809	299.347	-0.102921	299.347	-0.0108111
301.131	25.4186	301.131	14.6373	301.131	8.41993	301.131	4.55959	301.131	2.31402	301.131	0.774627	301.131	-0.152417	301.131	-0.0136765
302.915	23.0999	302.915	13.1263	302.915	7.40467	302.915	3.89976	302.915	1.8883	302.915	0.538981	302.915	-0.205517	302.915	-0.0176787
304.698	20.9457	304.698	11.707	304.698	6.44202	304.698	3.26753	304.698	1.47568	304.698	0.30668	304.698	-0.26096	304.698	-0.0224473
306.482	19.0093	306.482	10.4138	306.482	5.55489	306.482	2.67767	306.482	1.08565	306.482	0.0829573	306.482	-0.317493	306.482	-0.0276228
308.266	17.3087	308.266	9.25996	308.266	4.75286	308.266	2.13705	308.266	0.723156	308.266	-0.128972	308.266	-0.373914	308.266	-0.0329172
310.05	15.848	310.05	8.25015	310.05	4.03998	310.05	1.64926	310.05	0.391266	310.05	-0.326718	310.05	-0.429044	310.05	-0.0380716
311.834	14.6307	311.834	7.38896	311.834	3.42029	311.834	1.2179	311.834	0.0930523	311.834	-0.507894	311.834	-0.481703	311.834	-0.0428276
313.618	13.6609	313.618	6.68097	313.618	2.89786	313.618	0.846542	313.618	-0.168415	313.618	-0.670113	313.618	-0.530712	313.618	-0.0469265
315.402	12.9422	315.402	6.13078	315.402	2.47673	315.402	0.538784	315.402	-0.390067	315.402	-0.810987	315.402	-0.57489	315.402	-0.0501097
317.186	12.4785	317.186	5.74298	317.186	2.16095	317.186	0.298211	317.186	-0.568833	317.186	-0.92813	317.186	-0.613058	317.186	-0.0521186
318.97	12.2736	318.97	5.52218	318.97	1.95456	318.97	0.12841	318.97	-0.701644	318.97	-1.01916	318.97	-0.644037	318.97	-0.0526946
320.754	12.3313	320.754	5.47297	320.754	1.86162	320.754	0.0329701	320.754	-0.785429	320.754	-1.08168	320.754	-0.666647	320.754	-0.0515791
322.538	12.6555	322.538	5.59994	322.538	1.88618	322.538	0.015478	322.538	-0.817119	322.538	-1.1133	322.538	-0.679707	322.538	-0.0485134
324.322	13.2499	324.322	5.9077	324.322	2.03228	324.322	0.0795219	324.322	-0.793644	324.322	-1.11165	324.322	-0.68204	324.322	-0.0432391
326.106	14.1165	326.106	6.39958	326.106	2.30315	326.106	0.228134	326.106	-0.712315	326.106	-1.07457	326.106	-0.672548	326.106	-0.0355161
327.889	15.2318	327.889	7.06176	327.889	2.69063	327.889	0.456651	327.889	-0.575735	327.889	-1.00319	327.889	-0.651296	327.889	-0.025364
329.673	16.5536	329.673	7.86779	329.673	3.17823	329.673	0.754787	329.673	-0.39037	329.673	-0.901029	329.673	-0.619196	329.673	-0.0129916
331.457	18.0394	331.457	8.79098	331.457	3.74927	331.457	1.11213	331.457	-0.162775	331.457	-0.77167	331.457	-0.577181	331.457	0.00138785
333.241	19.6467	333.241	9.8046	333.241	4.38706	333.241	1.51825	333.241	0.100495	333.241	-0.61869	333.241	-0.526181	333.241	0.0175611
335.025	21.3328	335.025	10.882	335.025	5.07494	335.025	1.96275	335.025	0.392885	335.025	-0.445668	335.025	-0.467129	335.025	0.0353148
336.809	23.0552	336.809	11.9963	336.809	5.79621	336.809	2.43521	336.809	0.707839	336.809	-0.256182	336.809	-0.400957	336.809	0.0544358
338.593	24.7714	338.593	13.121	338.593	6.5342	338.593	2.92521	338.593	1.0388	338.593	-0.0538108	338.593	-0.328596	338.593	0.0747109
340.377	26.4387	340.377	14.2293	340.377	7.27224	340.377	3.42233	340.377	1.37922	340.377	0.157867	340.377	-0.250977	340.377	0.0959267
342.161	28.0147	342.161	15.2945	342.161	7.99363	342.161	3.91617	342.161	1.72254	342.161	0.375273	342.161	-0.169034	342.161	0.11787
343.945	29.4566	343.945	16.2899	343.945	8.68171	343.945	4.39631	343.945	2.0622	343.945	0.59483	343.945	-0.0836965	343.945	0.140328
345.729	30.7229	345.729	17.1892	345.729	9.32006	345.729	4.85249	345.729	2.39175	345.729	0.813003	345.729	0.00411062	345.729	0.163089
347.513	31.7995	347.513	17.983	347.513	9.90228	347.513	5.28034	347.513	2.70817	347.513	1.02794	347.513	0.0937599	347.513	0.186023
349.296	32.7082	349.296	18.6833	349.296	10.4347	349.296	5.68298	349.296	3.01287	349.296	1.23993	349.296	0.185	349.296	0.209102
351.08	33.473	351.08	19.3034	351.08	10.9243	351.08	6.06402	351.08	3.30751	351.08	1.44938	351.08	0.277603	351.08	0.232307
352.864	34.1178	352.864	19.8568	352.864	11.3784	352.864	6.42705	352.864	3.59377	352.864	1.65673	352.864	0.371343	352.864	0.255615
354.648	34.6667	354.648	20.3567	354.648	11.804	354.648	6.77568	354.648	3.87334	354.648	1.86239	354.648	0.465991	354.648	0.279006
356.432	35.1437	356.432	20.8165	356.432	12.2082	356.432	7.1135	356.432	4.14788	356.432	2.06679	356.432	0.561321	356.432	0.30246
358.216	35.5727	358.216	21.2496	358.216	12.5982	358.216	7.44413	358.216	4.41906	358.216	2.27034	358.216	0.657106	358.216	0.325956
360	35.9776	360	21.6694	360	12.981	360	7.77115	360	4.68857	360	2.47347	360	0.753118	360	0.349472

**Table S5:** CCSD(T)-F12 potentials depicted in Figures 4 and 5.

**(1A-CO<sub>2</sub>)<sub>a</sub>**

2.43	0.41
2.47	-0.75
2.57	-2.81
2.67	-3.97
2.77	-4.53
2.79	-4.59
2.82	-4.65
2.84	-4.68
2.86	-4.7
2.87	-4.7
2.88	-4.7
2.9	-4.7
2.92	-4.69
2.94	-4.68
2.97	-4.64
3.07	-4.43
3.17	-4.14
3.27	-3.81
3.37	-3.46658
3.47	-3.11624
3.57	-2.78263
3.67	-2.47278
3.77	-2.1903
3.87	-2.00102
4.07	-1.59165
4.37	-1.13995
4.57	-0.921384
4.87	-0.680546
5.37	-0.428551
5.87	-0.282806
6.37	-0.194063
6.87	-0.137625
7.37	-0.100408
7.87	-0.0750438
8.37	-0.0750438
8.87	-0.0445406

**(1A-CO<sub>2</sub>)<sub>b</sub>**

2.37	0.6
2.4	-0.12
2.44	-0.94
2.54	-2.41
2.64	-3.25
2.74	-3.67
2.76	-3.72
2.78	-3.75
2.8	-3.78
2.83	-3.8
2.84	-3.81
2.86	-3.81
2.88	-3.81
2.92	-3.79
2.94	-3.77
3.04	-3.62
3.14	-3.4
3.24	-3.14
3.34	-2.88
3.37	-2.8
3.4	-2.72
3.44	-2.62
3.54	-2.37
3.64	-2.14
3.74	-1.93
3.84	-1.73
3.94	-1.56
4.34	-1.03
4.84	-0.65
5.34	-0.42
5.84	-0.29
6.34	-0.21
6.84	-0.15

7.34	-0.12
7.84	-0.09
8.34	-0.07
8.84	-0.06

**(IA-CO<sub>2</sub>)<sub>c</sub>**

2.56	0.2
2.58	-0.157084
2.61	-0.646749
2.64	-1.07559
2.67	-1.44951
2.7	-1.77385
2.73	-2.05344
2.76	-2.2927
2.79	-2.49562
2.82	-2.66583
2.85	-2.80667
2.88	-2.92115
2.91	-3.01205
2.94	-3.08191
2.97	-3.13304
3	-3.16756
3.03	-3.18741
3.06	-3.19436
3.09	-3.19
3.12	-3.17579
3.15	-3.15303
3.18	-3.12291
3.21	-3.08649
3.24	-3.04472
3.27	-2.99844
3.3	-2.94841
3.33	-2.89531
3.36	-2.8397
3.39	-2.78215
3.42	-2.72308
3.45	-2.66292
3.48	-2.60202
3.51	-2.54069
3.54	-2.4792
3.57	-2.41781
3.6	-2.35671
3.63	-2.29607
3.66	-2.23607
3.69	-2.17682
3.72	-2.11845
3.82	-1.94657
3.92	-1.75253
4.02	-1.5789
4.12	-1.42412
4.22	-1.28645
4.32	-1.16412
4.42	-1.05545
4.62	-0.872878
4.82	-0.727729
5.32	-0.47857
5.82	-0.32894
6.32	-0.234525
6.82	-0.172396
7.32	-0.129995
7.82	-0.100163

**(IA-CO<sub>2</sub>)<sub>d</sub>**

2.6	0.279242
2.63	-0.0880019
2.64	-0.423468
2.74	-1.69467
2.84	-2.44199
2.94	-2.82835
2.96	-2.87337
2.98	-2.90957
3.01	-2.94887
3.04	-2.97215
3.07	-2.98145
3.11	-2.97515

3.14	-2.95852
3.19	-2.91219
3.24	-2.84743
3.34	-2.6803
3.44	-2.48507
3.54	-2.28016
3.64	-2.07733
3.74	-1.88369
3.84	-1.70318
3.94	-1.53762
4.04	-1.3875
4.14	-1.25243
4.2	-1.17824
4.54	-0.841979
5.04	-0.535008
5.54	-0.340185
6.04	-0.248663
6.54	-0.178972
7.04	-0.13236
7.54	-0.10015
8.04	-0.0772526
8.54	-0.0605986

**(1A-CO<sub>2</sub>)<sub>e</sub>**

2.73	-0.01
2.83	-1.38196
2.93	-2.16792
3.03	-2.58363
3.09	-2.70711
3.13	-2.74991
3.19	-2.76728
3.23	-2.75379
3.29	-2.70483
3.33	-2.65717
3.43	-2.5027
3.53	-2.31925
3.63	-2.12549
3.73	-1.93317
3.83	-1.74924
3.93	-1.57754
4.13	-1.27666
4.43	-0.928958
4.63	-0.755333
5.13	-0.463365
5.63	-0.296711
6.13	-0.197138
6.63	-0.134952
7.13	-0.0946911
7.63	-0.0678526

**(1B-CO<sub>2</sub>)<sub>a</sub>**

2.43	0.569716
2.47	-0.548587
2.57	-2.53073
2.67	-3.65168
2.72	-3.9825
2.77	-4.19859
2.82	-4.3228
2.87	-4.37395
2.92	-4.36749
2.97	-4.31603
3.07	-4.11726
3.17	-3.83918
3.27	-3.52279
3.37	-3.19522
3.47	-2.87402
3.57	-2.56974
3.67	-2.2887
3.77	-2.03339
3.87	-1.80429
3.97	-1.60047
4.07	-1.42018
4.27	-1.12165
4.37	-0.998944
4.57	-0.792588

4.77 -0.636928  
4.87 -0.575351  
5.37 -0.347684  
5.87 -0.219365  
6.37 -0.14353  
6.87 -0.0968623  
7.37 -0.0671372  
7.87 -0.0476154  
8.37 -0.0344628  
8.87 -0.025389

**(IB-CO<sub>2</sub>)<sub>b</sub>**

2.82 0.0313566  
2.92 -1.13958  
3.02 -1.83446  
3.07 -2.05092  
3.12 -2.20006  
3.17 -2.29419  
3.22 -2.34384  
3.27 -2.35789  
3.32 -2.34388  
3.37 -2.30812  
3.42 -2.25581  
3.52 -2.11796  
3.62 -1.9559  
3.72 -1.78595  
3.82 -1.61818  
3.92 -1.4584  
4.02 -1.30977  
4.12 -1.17374  
4.22 -1.05061  
4.42 -0.841358  
4.52 -0.756776  
4.72 -0.606676  
4.92 -0.493436  
5.22 -0.363246  
5.72 -0.227773  
6.22 -0.148826  
6.72 -0.100552  
7.22 -0.0698355  
7.72 -0.049636  
8.22 -0.0360002  
8.72 -0.0265876

**(IB-CO<sub>2</sub>)<sub>c</sub>**

2.34 0.0986695  
2.37 -0.116485  
2.4 -0.303244  
2.43 -0.464564  
2.46 -0.603118  
2.49 -0.721366  
2.52 -0.834788  
2.55 -0.916559  
2.58 -0.984235  
2.61 -1.03941  
2.64 -1.08355  
2.67 -1.11793  
2.7 -1.14374  
2.73 -1.162  
2.76 -1.17366  
2.79 -1.17956  
2.82 -1.18046  
2.85 -1.17705  
2.88 -1.1699  
2.91 -1.15954  
2.94 -1.14648  
2.97 -1.13112  
3 -1.11383  
3.03 -1.09497  
3.06 -1.0748  
3.09 -1.0536  
3.12 -1.0316  
3.15 -1.00899  
3.18 -0.985955  
3.21 -0.96263

3.24	-0.939174
3.27	-0.915699
3.3	-0.892299
3.33	-0.869044
3.36	-0.84479
3.39	-0.823279
3.42	-0.800877
3.45	-0.778877
3.48	-0.757284
3.51	-0.73615
3.54	-0.715473
3.57	-0.695286
3.6	-0.675608
3.67	-0.631663
3.77	-0.573738
3.87	-0.521435
3.97	-0.474409
4.07	-0.432278
4.17	-0.394584
4.3	-0.351499
4.43	-0.314181
4.8	-0.234525
5.32	-0.172396
5.82	-0.129995
6.32	-0.100163
6.82	-0.0786081
7.32	-0.0626882

**(2A-CO<sub>2</sub>)<sub>a</sub>**

2.41	0.3814
2.45	-0.769822
2.55	-2.81386
2.65	-3.97417
2.75	-4.54273
2.78	-4.63045
2.82	-4.70134
2.85	-4.72481
2.88	-4.72663
2.92	-4.69982
2.95	-4.6615
3	-4.56916
3.05	-4.44877
3.15	-4.15176
3.25	-3.81419
3.35	-3.46529
3.45	-3.13189
3.55	-2.80801
3.65	-2.50837
3.75	-2.23565
3.85	-1.98459
3.95	-1.77141
4.05	-1.57275
4.15	-1.40566
4.35	-1.11803
4.55	-0.897959
4.85	-0.655929
5.35	-0.404141
5.85	-0.26009
6.35	-0.173619
6.85	-0.119522
7.35	-0.0844941
7.85	-0.0611068
8.35	-0.0450865
8.85	-0.0338667

**(2A-CO<sub>2</sub>)<sub>b</sub>**

2.39	-0.0912022
2.43	-0.983288
2.53	-2.58205
2.63	-3.50304
2.68	-3.77954
2.73	-3.96248
2.78	-4.06937
2.83	-4.11483
2.88	-4.11112



2.93	-4.06839
2.98	-3.99516
3.03	-3.89845
3.13	-3.65714
3.23	-3.38025
3.33	-3.09154
3.43	-2.80657
3.53	-2.53483
3.63	-2.28164
3.73	-2.04952
3.83	-1.83917
3.93	-1.65007
4.03	-1.48107
4.13	-1.33059
4.33	-1.07833
4.83	-0.657749
5.33	-0.420839
5.83	-0.281068
6.33	-0.194622
6.83	-0.138931
7.33	-0.101769
7.83	-0.0762298
8.33	-0.0582203
8.83	-0.0452246

**(2A-CO<sub>2</sub>)<sub>c</sub>**

2.8		0
2.83	-1.38196	
2.93	-2.16792	
3.03	-2.58363	
3.09	-2.70711	
3.13	-2.74991	
3.19	-2.76728	
3.23	-2.75379	
3.29	-2.70483	
3.33	-2.65717	
3.43	-2.5027	
3.53	-2.31925	
3.63	-2.12549	
3.73	-1.93317	
3.83	-1.74924	
3.93	-1.57754	
4.13	-1.27666	
4.43	-0.928958	
4.63	-0.755333	
5.13	-0.463365	
5.63	-0.296711	
6.13	-0.197138	
6.63	-0.134952	
7.13	-0.0946911	
7.63	-0.0678526	
8.13	-0.0678526	
8.63	-0.0495356	

**(2A-CO<sub>2</sub>)<sub>d</sub>**

2.73	-0.0591427
2.83	-1.38196
2.93	-2.16792
3.03	-2.58363
3.09	-2.70711
3.13	-2.74991
3.19	-2.76728
3.23	-2.75379
3.29	-2.70483
3.33	-2.65717
3.43	-2.5027
3.53	-2.31925
3.63	-2.12549
3.73	-1.93317
3.83	-1.74924
3.93	-1.57754
4.13	-1.27666
4.43	-0.928958
4.63	-0.755333
5.13	-0.463365

5.63	-0.296711
6.13	-0.197138
6.63	-0.134952
7.13	-0.0946911
7.63	-0.0678526
8.13	-0.0678526
8.63	-0.0495356

**(2B-CO<sub>2</sub>)<sub>a</sub>**

2.39	-0.404536
2.42	-1.07292
2.52	-2.7065
2.62	-3.64404
2.67	-3.92432
2.72	-4.10916
2.77	-4.21669
2.82	-4.26207
2.87	-4.25782
2.92	-4.21433
2.97	-4.14016
3.02	-4.04243
3.12	-3.79856
3.22	-3.51825
3.32	-3.22533
3.42	-2.93546
3.52	-2.65839
3.62	-2.39971
3.72	-2.16216
3.82	-1.94657
3.92	-1.75253
4.02	-1.5789
4.12	-1.42412
4.22	-1.28645
4.32	-1.16412
4.42	-1.05545
4.62	-0.872878
4.82	-0.727729
5.32	-0.47857
5.82	-0.32894
6.32	-0.234525
6.82	-0.172396
7.32	-0.129995
7.82	-0.100163
8.32	-0.0786081
8.82	-0.0626882

**(2B-CO<sub>2</sub>)<sub>b</sub>**

2.49	0.0685807
2.5	-0.269076
2.53	-0.860547
2.56	-1.37595
2.59	-1.82308
2.62	-2.20849
2.65	-2.53864
2.68	-2.81925
2.71	-3.05543
2.74	-3.25187
2.77	-3.41276
2.8	-3.54197
2.83	-3.64296
2.86	-3.7189
2.89	-3.77263
2.92	-3.80678
2.95	-3.82369
2.98	-3.82551
3.01	-3.81416
3.04	-3.79125
3.07	-3.75862
3.1	-3.71752
3.13	-3.66923
3.16	-3.61487
3.19	-3.55546
3.82	-1.94657
3.92	-1.75253
4.02	-1.5789

4.12	-1.42412
4.22	-1.28645
4.32	-1.16412
4.42	-1.05545
4.62	-0.872878
4.82	-0.727729
5.32	-0.47857
5.82	-0.32894
6.32	-0.234525
6.82	-0.172396
7.32	-0.129995
7.82	-0.100163
8.32	-0.0786081
8.82	-0.0626882

**(2B-CO<sub>2</sub>)<sub>c</sub>**

2.6	0.545895
2.64	-0.294685
2.68	-0.99794
2.7	-1.30363
2.73	-1.71026
2.77	-2.16552
2.82	-2.61298
2.86	-2.88775
2.9	-3.09955
2.94	-3.25727
2.97	-3.34484
3.02	-3.44097
3.05	-3.48028
3.1	-3.49064
3.15	-3.46626
3.2	-3.41467
3.25	-3.34218
3.3	-3.25397
3.35	-3.15431
3.4	-3.04668
3.45	-2.93388
3.55	-2.70141
3.65	-2.47
3.85	-2.03932
4	-1.75733
4.3	-1.30526
4.6	-0.979968
4.9	-0.747464
5.2	-0.579787
5.5	-0.456971
5.8	-0.36538
6.1	-0.295839
6.5	-0.227089
7	-0.167037

**(2B-CO<sub>2</sub>)<sub>d</sub>**

1.72	-0.216899
1.82	-1.46476
1.92	-2.16961
1.96	-2.34382
1.98	-2.4127
2.02	-2.51909
2.04	-2.55835
2.08	-2.61304
2.12	-2.64049
2.17	-2.64382
2.22	-2.62002
2.27	-2.57562
2.32	-2.51587
2.42	-2.36673
2.52	-2.19762
2.62	-2.02397
2.72	-1.85473
2.82	-1.69468
2.92	-1.54604
3.02	-1.40977
3.12	-1.28601
3.22	-1.17438
3.42	-0.98438

3.62	-0.832171
3.82	-0.709807
4.12	-0.568015
4.62	-0.405929
5.12	-0.300332
5.62	-0.228275
6.12	-0.177365
6.62	-0.140349
7.12	-0.112876
7.62	-0.0918987
8.12	-0.0757278
8.62	-0.063096

**(2B-CO<sub>2</sub>)<sub>e</sub>**

2.6	0.545895
2.64	-0.294685
2.68	-0.99794
2.7	-1.30363
2.73	-1.71026
2.77	-2.16552
2.82	-2.61298
2.86	-2.88775
2.9	-3.09955
2.94	-3.25727
2.97	-3.34484
3.02	-3.44097
3.05	-3.48028
3.1	-3.49064
3.15	-3.46626
3.2	-3.41467
3.25	-3.34218
3.3	-3.25397
3.35	-3.15431
3.4	-3.04668
3.45	-2.93388
3.55	-2.70141
3.65	-2.47
3.85	-2.03932
4	-1.75733
4.3	-1.30526
4.6	-0.979968
4.9	-0.747464
5.2	-0.579787
5.5	-0.456971
5.8	-0.36538
6.1	-0.295839
6.5	-0.227089
7	-0.167037
7.5	-0.125608
8	-0.0962787