

Dynamical Electron Correlation and the Chemical Bond. III. Covalent Bonds in the A_2 Molecules ($A = C-F$)

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ABSTRACT. For most molecules the Spin-Coupled Generalized Valence Bond (SCGVB) wavefunction accounts for the effects of non-dynamical electron correlation. The remaining errors in the prediction of molecular properties and the outcomes of molecular processes are then solely due to dynamical electron correlation. In this article we extend our previous studies of the effects of dynamical electron correlation on the potential energy curves and spectroscopic constants of the AH and AF ($A = B-F$) molecules to the homonuclear diatomic molecules, A_2 ($A = C-F$). At large R the magnitude of $\Delta E_{DEC}(R)$, the correlation energy of the molecule relative to that in the atoms, increases nearly exponentially with decreasing R , just as we found in the AH and AF molecules. But, as R continues to decrease the rate of increase in the magnitude of $\Delta E_{DEC}(R)$ slows, eventually leading to a minimum for C_2-O_2 . Examination of the SCGVB wavefunction for the N_2 molecule around the minimum in $\Delta E_{DEC}(R)$ did not reveal a clear cause for this puzzling behavior. As before, the changes in $\Delta E_{DEC}(R)$ around R_e were found to have an uneven effect on the spectroscopic constants of the A_2 molecules.

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	C2					
	SCGVB	vCAS(1)	VCASCI(1)	vCASCI(1)+Q	CCSD(T)	Expt'l
Ee(hartrees)	-75.594679	-75.629859	-75.794748	-75.804474	-75.802143	
E[Re(vcasci3)]	-75.594662	-75.629760	-75.794748	-75.804458		
Re(Å)	1.244	1.256	1.248	1.248	1.246	1.2425
ωe(cm-1)	1842.6	1816.8	1841.2	1837.4	1854.0	1854.71
ωexe(cm-1)	14.54	12.53	13.53	13.80	13.19	13.34
De(kcal/mol)	112.6	137.2	144.1	143.5	143.6	145.2
D0(kca/mol)	110.0	134.6	141.5	140.9	141.0	

	N2					
	SCGVB	vCAS3	VCASCI3	vCASCI3+Q	CCSD(T)	Expt'l
	-109.073564	-109.139923	-109.392392	-109.407111	-109.407243	
	-109.073489	-109.139901	-109.392392	-109.407110		
	1.096	1.104	1.101	1.101	1.100	1.09768
	2369.4	2338.6	2350.1	2342.4	2354.1	2358.57
	15.63	13.27	13.65	13.73	13.41	14.324
	171.4	213.0	225.1	224.1	224.1	228.4
	168.0	209.7	221.7	220.7	220.7	

	O2					
	SCGVB(2csf)	vCAS3	VCASCI3	vCASCI3+Q	CCSD(T)	Expt'l
Ee(hartrees)	-149.729913	-149.769375	-150.147042	-150.175050	-150.177985	
E[Re(vcasci3)]	-149.729827	-149.769302	-150.147042	-150.175042		
Re(Å)	1.200	1.215	1.208	1.211	1.208	1.20752
ωe(cm-1)	1579.3	1547.6	1584.0	1573.2	1600.5	1580.19
ωexe(cm-1)	26.90	11.67	10.99	10.94	17.01	11.98
De(kcal/mol)	68.6	95.0	116.4	118.3	118.0	120.2
D0(kca/mol)	66.3	92.8	114.2	116.1	115.8	

	F2					
	SCGVB	vCAS3	VCASCI3	vCASCI3+Q	CCSD(T)	Expt'l
	-198.844910	-198.848866	-199.324611	-199.358788	-199.365736	
	-198.843909	-198.848110	-199.324611	-199.358788		
	1.467	1.459	1.415	1.414	1.413	1.41193
	698.8	733.4	895.9	911.8	921.4	916.64
	19.82	19.83	13.05	12.45	12.25	11.236
	16.6	19.1	34.8	37.2	37.8	38.3
	15.6	18.1	33.5	35.9	36.5	

Changes in Spectroscopic Constants Due to DEC

	C2	N2	O2	F2
ΔEe(H)	-0.200069	-0.318828	-0.417129	-0.479701
ΔE(kcal/mol)	-125.5452	-200.0676	-261.7525	-301.0170
ΔRe(Å)	0.003	0.005	0.008	-0.053
Δωe(cm-1)	-1.4	-19.3	4.6	197.1
ΔDE(kcal/mol)	31.5	53.7	47.9	18.1

C2: RHF, CCSD(T), SCGVB, vCAS and vCASI ENERGIES

R(Å)	E(R=∞)		R(R=∞)		E(R=20.00)		F(R=20.00)		E(R=20.00)		E(R=20.00)		E(R=20.00)	
	-75.376646		-75.573271		-75.41520527		-75.41122250		-75.56511440		-75.41122246		-75.56511436	
	E(RHF)	ΔE(RHF)	E[CCSD(T)]	ΔE[CCSD(T)]	SCGVB	ΔE(SCGVB)	vCAS(3State)	ΔE1(vCAS)	E1(vCASI)	ΔE1(vCASI)	ΔE2(vCAS)	E2(vCAS)	ΔE2(vCASI)	
0.918					-75.28202758	83.5703	-75.30350129	67.5961	-75.47930335	53.8473	-75.10873462	189.8140	-75.29758730	
0.928					-75.30799699	67.2742	-75.32986582	51.0521	-75.50522110	37.5836	-75.13644556	172.4251	-75.32446959	
0.938					-75.33230968	52.0178	-75.35457646	35.5459	-75.52950010	22.3483	-75.16264244	155.9863	-75.34985328	
0.948					-75.35504949	37.7483	-75.37771696	21.0250	-75.55222321	8.0893	-75.18741678	140.4402	-75.37383306	
0.958					-75.37629627	24.4158	-75.39936717	7.4393	-75.57346926	-5.2428	-75.21085510	125.7324	-75.39649874	
0.968					-75.39612608	11.9724	-75.41960326	-5.2590	-75.59331334	-17.6951	-75.23303867	111.8120	-75.41793479	
0.978					-75.41461137	0.3727	-75.43849782	-17.1155	-75.61182688	-29.3125	-75.25404322	98.6315	-75.43821986	
0.988					-75.43182109	-10.4266	-75.45612004	-28.1736	-75.62907786	-40.1377	-75.27393868	86.1469	-75.45742636	
0.998					-75.44782092	-20.4666	-75.47253578	-38.4747	-75.64513096	-50.2112	-75.29278910	74.3181	-75.47562012	
1.008					-75.46267338	-29.7867	-75.48780775	-48.0580	-75.66004773	-59.5716	-75.31065267	63.1085	-75.49286032	
1.018					-75.47643797	-38.4241	-75.50199556	-56.9610	-75.67388674	-68.2557	-75.32758185	52.4853	-75.50919962	
1.028					-75.48917136	-46.4144	-75.51515589	-65.2192	-75.68670369	-76.2984	-75.34362374	42.4188	-75.52468449	
1.038					-75.50092747	-53.7915	-75.52734254	-72.8664	-75.69855164	-83.7331	-75.35882055	32.8827	-75.53935585	
1.048					-75.51175766	-60.5876	-75.53860662	-79.9348	-75.70948100	-90.5914	-75.37321019	23.8531	-75.55324980	
1.058					-75.52171079	-66.8332	-75.54899663	-86.4546	-75.71953980	-96.9034	-75.38682692	15.3084	-75.56639847	
1.068					-75.53083340	-72.5578	-75.55855858	-92.4548	-75.72877374	-102.6978	-75.39970201	7.2292	-75.57883087	
1.088					-75.54676215	-82.5532	-75.57537083	-103.0047	-75.74493884	-112.8416	-75.42334113	-7.6046	-75.60165156	
1.108					-75.55987343	-90.7807	-75.58936678	-111.7872	-75.75829957	-121.2255	-75.44433968	-20.7814	-75.62237921	
1.128					-75.57046602	-97.4276	-75.60083800	-118.9855	-75.76914875	-128.0335	-75.46289275	-32.4236	-75.64293211	
1.148					-75.57881080	-102.6640	-75.61004771	-124.7647	-75.77751688	-133.4319	-75.47918530	-42.6473	-75.66076770	
1.168	-75.39723320	-12.9185	-75.79211068	-137.3239	-75.58515348	-106.6441	-75.61723389	-129.2741	-75.78434880	-137.5717	-75.49339484	-51.5640	-75.67615545	
1.188	-75.40158833	-15.6513	-75.79682935	-140.2849	-75.58971692	-109.5077	-75.62261195	-132.6489	-75.78915814	-140.5896	-75.50569172	-59.2804	-75.68933935	
1.208	-75.40433666	-17.3759	-75.79995728	-142.2477	-75.59270329	-111.3817	-75.62637712	-135.0116	-75.79237748	-142.6098	-75.51730082	-66.5652	-75.70054032	
1.228	-75.40563958	-18.2061	-75.80167318	-143.3245	-75.59429604	-112.3812	-75.62870648	-136.4733	-75.79418635	-143.7448	-75.52736968	-72.8835	-75.70995849	
1.248	-75.40572159	-18.2450	-75.80213907	-143.6168	-75.59466160	-112.6106	-75.62976072	-137.1348	-75.79474780	-144.0972	-75.53580678	-78.1779	-75.71777514	
1.268	-75.40467185	-17.5863	-75.80149586	-143.2132	-75.59395097	-112.1646	-75.62968577	-137.0878	-75.79421004	-143.7597	-75.54277910	-82.5531	-75.72415458	
1.288	-75.40264544	-16.3147	-75.79989620	-142.2094	-75.59230113	-111.1294	-75.62861420	-136.4154	-75.79270793	-142.8171	-75.54843776	-86.1039	-75.72924571	
1.308	-75.39976466	-14.5070	-75.79744121	-140.6689	-75.58983630	-109.5826	-75.62666645	-135.1931	-75.79036425	-141.3464	-75.55291958	-88.9163	-75.73318355	
1.328	-75.39614006	-12.2325	-75.79424230	-138.6615	-75.58666910	-107.5952	-75.62395204	-133.4898	-75.78729097	-139.4179	-75.55634848	-91.0680	-75.73609051	
1.348					-75.58290157	-105.2310	-75.62057059	-131.3679	-75.78359044	-137.0958	-75.55883673	-92.6294	-75.73807757	
1.368					-75.57862610	-102.5481	-75.61661276	-128.8844	-75.77935640	-134.4389	-75.56048604	-93.6643	-75.73924539	
1.388					-75.57392628	-99.5990	-75.61216113	-126.0909	-75.77467509	-131.5013	-75.56138863	-94.2307	-75.73968522	
1.408					-75.56887763	-96.4309	-75.60729106	-123.0349	-75.76962629	-128.3332	-75.56162803	-94.3809	-75.73947979	
1.428					-75.56354834	-93.0867	-75.60207143	-119.7595	-75.76428438	-124.9811	-75.56127998	-94.1625	-75.73870406	
1.448					-75.55799987	-89.6050	-75.59656539	-116.3044	-75.75871941	-121.4890	-75.56041308	-93.6185	-75.73742594	
1.468					-75.55228750	-86.0204	-75.59083116	-112.7062	-75.75299833	-117.8990	-75.55908948	-92.7880	-75.73570695	
1.488					-75.54646089	-82.3642	-75.58492279	-108.9986	-75.74718606	-114.2517	-75.55736549	-91.7062	-75.73360273	
1.508					-75.54056456	-78.6642	-75.57889102	-105.2136	-75.74134649	-110.5873	-75.55529203	-90.4050	-75.73116361	
1.528					-75.53463828	-74.9454	-75.57278426	-101.3816	-75.73554263	-106.9454	-75.55291521	-88.9136	-75.72843507	
1.548					-75.52871753	-71.2300	-75.56664982	-97.5321	-75.72983539	-103.3640	-75.55027670	-87.2579	-75.72545816	
1.568					-75.52283382	-67.5379	-75.56053524	-93.6952	-75.72427981	-99.8778	-75.54741416	-85.4616	-75.72226991	
1.588					-75.51701507	-63.8866	-75.55448993	-89.9017	-75.71891872	-96.5137	-75.54436157	-83.5461	-75.71890367	
1.608					-75.51128587	-60.2915	-75.54856636	-86.1846	-75.71538946	-94.2990	-75.54114961	-81.5305	-75.71377553	
1.628					-75.50566780	-56.7661	-75.54281986	-82.5786	-75.71175421	-92.0179	-75.53780592	-79.4323	-75.70885105	
1.648					-75.50017965	-53.3222	-75.53730438	-79.1176	-75.70802214	-89.6760	-75.53435538	-77.2671	-75.70412694	
1.668					-75.49483768	-49.9701	-75.53206231	-75.8281	-75.70421493	-87.2869	-75.53082038	-75.0488	-75.69957448	
1.688					-75.48965579	-46.7184	-75.52722106	-72.7902	-75.70035199	-84.8629	-75.52711101	-72.7212	-75.69516351	
1.708					-75.48464570	-43.5745	-75.52357547	-70.5026	-75.69645066	-82.4148	-75.52243617	-69.7877	-75.69086816	
1.728					-75.47981712	-40.5446	-75.51989984	-68.1961	-75.69252643	-79.9523	-75.51799975	-67.0038	-75.68666895	
1.748					-75.47517787	-37.6334	-75.51620870	-65.8798	-75.68859308	-77.4841	-75.51375641	-64.3410	-75.68255252	
1.768					-75.47073402	-34.8448	-75.51251507	-63.5621	-75.68466290	-75.0178	-75.50966626	-61.7744	-75.67851055	
1.788					-75.46648997	-32.1816	-75.50883062	-61.2500	-75.68074682	-72.5605	-75.50569971	-59.2854	-75.67453840	
1.808					-75.46244857	-29.6456	-75.50516578	-58.9503	-75.67685452	-70.1180	-75.50183706	-56.8615	-75.67063401	
1.828					-75.45861120	-27.2376	-75.50152989	-56.6688	-75.67299461	-67.6959	-75.49806620	-54.4953	-75.66679705	
1.848					-75.45497784	-24.9577	-75.49793131	-54.4106	-75.66917471	-65.2988	-75.49438030	-52.1823	-75.66302830	
1.868					-75.45154721	-22.8049	-75.49437752	-52.1806	-75.66540158	-62.9312	-75.49077603	-49.9206	-75.65932919	
1.888					-75.44831685	-20.7778	-75.49087522	-49.9828	-75.66168118	-60.5966	-75.48725224	-47.7094	-75.65570153	
1.908					-75.44528322	-18.8742	-75.48743040	-47.8212	-75.65801880	-58.2984	-75.48380920	-45.5489	-75.65214728	
1.928					-75.44244181	-17.0912	-75.48404845	-45.6990	-75.65441909	-56.0396	-75.48044799	-43.4397	-75.64866845	
1.948					-75.43978733	-15.4255	-75.48073419	-43.6193	-75.65088619	-53.8226	-75.47717016	-41.3828	-75.64526699	
1.968					-75.43731378	-13.8733	-75.47749196	-41.5847	-75.64742371	-51.6499	-75.47397749	-39.3794	-75.64194475	
1.988					-75.43501461	-12.4306	-75.47432564	-39.5978	-75.64403485	-49.5233	-75.47087184	-37.4306	-75.63870341	
2.008					-75.43288288	-11.0929	-75.47123871	-37.6607	-75.64072242	-47.4448	-75.46785506	-35.5375	-75.63554453	
2.028					-75.43091135	-9.8557	-75.46823429	-35.7754	-75.63748888	-45.4157	-75.46492890	-33.7013	-75.63246945	
2.048					-75.42909262	-8.7144	-75.46531515	-33.9437	-75.63433636	-43.4374	-75.46209497	-31.9230	-75.62947935	

2.068		-75.42741919	-7.6644	-75.46248372	-32.1669	-75.63126671	-41.5112	-75.45935471	-30.2034	-75.62657524
2.088		-75.42588354	-6.7007	-75.45974215	-30.4465	-75.62828151	-39.6380	-75.45670934	-28.5435	-75.62375791
2.108		-75.42447816	-5.8188	-75.45709225	-28.7837	-75.62538210	-37.8186	-75.45415989	-26.9436	-75.62102799
2.128		-75.42319558	-5.0140	-75.45453553	-27.1793	-75.62256958	-36.0537	-75.45170711	-25.4045	-75.61838591
2.148		-75.42202838	-4.2816	-75.45207320	-25.6342	-75.61984480	-34.3439	-75.44935152	-23.9264	-75.61583194
2.168		-75.42096920	-3.6169	-75.44970615	-24.1489	-75.61720843	-32.6895	-75.44709335	-22.5093	-75.61336612
2.188		-75.42001079	-3.0155	-75.44743495	-22.7237	-75.61466091	-31.0909	-75.44493254	-21.1534	-75.61098834
2.208		-75.41914603	-2.4729	-75.44525983	-21.3588	-75.61220247	-29.5482	-75.44286873	-19.8583	-75.60869829
2.228		-75.41836798	-1.9846	-75.44318073	-20.0541	-75.60983313	-28.0614	-75.44090128	-18.6237	-75.60649549
2.278		-75.41675872	-0.9748	-75.43839943	-17.0538	-75.60429792	-24.5880	-75.43639714	-15.7974	-75.60136532
2.328		-75.41555330	-0.2184	-75.43419916	-14.4181	-75.59930951	-21.4578	-75.43246523	-13.3300	-75.59676037
2.378		-75.41466835	0.3369	-75.43055232	-12.1296	-75.59485168	-18.6604	-75.42907164	-11.2005	-75.59265870
2.428		-75.41403470	0.7345	-75.42742086	-10.1646	-75.59090082	-16.1812	-75.42617365	-9.3820	-75.58903252
2.478		-75.41359634	1.0096	-75.42475883	-8.9492	-75.58742669	-14.0012	-75.42372236	-7.8438	-75.58584911
2.528		-75.41330858	1.1902	-75.42251548	-7.0865	-75.58439363	-12.0979	-75.42166574	-6.5533	-75.58307207
2.578		-75.41313599	1.2985	-75.42063839	-5.9086	-75.58176211	-10.4466	-75.41995150	-5.4776	-75.58066267
2.628		-75.41305059	1.3521	-75.41907629	-4.9283	-75.57949063	-9.0212	-75.41852956	-4.5853	-75.57858143
2.678		-75.41303023	1.3649	-75.41778120	-4.1156	-75.57753756	-7.7957	-75.41735378	-3.8475	-75.57678957
2.728		-75.41305738	1.3478	-75.41670979	-3.4433	-75.57586272	-6.7447	-75.41638302	-3.2383	-75.57525024
2.778		-75.41311807	1.3097	-75.41582408	-2.8875	-75.57442864	-5.8448	-75.41558156	-2.7354	-75.57392938
2.828		-75.41320112	1.2576	-75.41509149	-2.4278	-75.57320130	-5.0746	-75.41491901	-2.3196	-75.57279624
2.878		-75.41329761	1.1971	-75.41448461	-2.0470	-75.57215046	-4.4152	-75.41436999	-1.9751	-75.57182360
2.928		-75.41340057	1.1325	-75.41398069	-1.7308	-75.57124972	-3.8500	-75.41391355	-1.6887	-75.57098770
2.978		-75.41350497	1.0670	-75.41356100	-1.4674	-75.57047634	-3.3647	-75.41353258	-1.4496	-75.57026805
3.028		-75.41360752	1.0026	-75.41321319	-1.2492	-75.56981090	-2.9471	-75.41321027	-1.2474	-75.56964718
3.078		-75.41370631	0.9406	-75.41294415	-1.0804	-75.56923698	-2.5870	-75.41291606	-1.0628	-75.56911024
3.128		-75.41380032	0.8816	-75.41271644	-0.9375	-75.56874071	-2.2755	-75.41266833	-0.9073	-75.56864469
3.178		-75.41388911	0.8259	-75.41252278	-0.8159	-75.56831045	-2.0056	-75.41245890	-0.7759	-75.56823997
3.228		-75.41397255	0.7735	-75.41235730	-0.7121	-75.56793643	-1.7709	-75.41228120	-0.6644	-75.56788720
3.278		-75.41405071	0.7245	-75.41221527	-0.6230	-75.56761044	-1.5663	-75.41212985	-0.5694	-75.56757891
3.328		-75.41412378	0.6786	-75.41209288	-0.5462	-75.56732562	-1.3876	-75.41200054	-0.4883	-75.56730884
3.378		-75.41419199	0.6358	-75.41198702	-0.4797	-75.56707618	-1.2310	-75.41188970	-0.4187	-75.56707169
3.428		-75.41425560	0.5959	-75.41189515	-0.4221	-75.56686298	-1.0973	-75.41179447	-0.3589	-75.56685725
3.478		-75.41431490	0.5587	-75.41181520	-0.3719	-75.56667896	-0.9818	-75.41171247	-0.3075	-75.56666473
3.528		-75.41437017	0.5240	-75.41174546	-0.3282	-75.56651640	-0.8798	-75.41164174	-0.2631	-75.56649513
3.578		-75.41442166	0.4917	-75.41168449	-0.2899	-75.56637255	-0.7895	-75.41158067	-0.2248	-75.56634548
3.628		-75.41446963	0.4616	-75.41163112	-0.2564	-75.56624508	-0.7095	-75.41152788	-0.1917	-75.56621326
3.678		-75.41451433	0.4336	-75.41158432	-0.2270	-75.56613196	-0.6385	-75.41148225	-0.1630	-75.56609622
3.728		-75.41455598	0.4074	-75.41154325	-0.2013	-75.56603144	-0.5755	-75.41144280	-0.1383	-75.56599266
3.778		-75.41459479	0.3831	-75.41150716	-0.1786	-75.56594201	-0.5193	-75.41140870	-0.1169	-75.56590078
3.828		-75.41463097	0.3604	-75.41147542	-0.1587	-75.56586234	-0.4693	-75.41137924	-0.0984	-75.56581925
3.878		-75.41466471	0.3392	-75.41144748	-0.1412	-75.56579129	-0.4248	-75.41135381	-0.0824	-75.56574680
3.928		-75.41469618	0.3195	-75.41142286	-0.1257	-75.56572783	-0.3849	-75.41133185	-0.0686	-75.56568236
3.978		-75.41472555	0.3010	-75.41140116	-0.1121	-75.56565710	-0.3493	-75.41131292	-0.0568	-75.56562500
4.028		-75.41475296	0.2838	-75.41138199	-0.1001	-75.56562030	-0.3175	-75.41129660	-0.0465	-75.56557387
4.078		-75.41477857	0.2678	-75.41136504	-0.0894	-75.56557476	-0.2889	-75.41128254	-0.0377	-75.56552826
4.128		-75.41480250	0.2527	-75.41135004	-0.0800	-75.56553388	-0.2632	-75.41127042	-0.0301	-75.56548752
4.178		-75.41482488	0.2387	-75.41133674	-0.0717	-75.56549714	-0.2402	-75.41126000	-0.0236	-75.56545109
4.228		-75.41484583	0.2256	-75.41132493	-0.0643	-75.56546406	-0.2194	-75.41125103	-0.0179	-75.56541848
4.278		-75.41486544	0.2132	-75.41131444	-0.0577	-75.56543425	-0.2007	-75.41124331	-0.0131	-75.56538925
4.328		-75.41488382	0.2017	-75.41130509	-0.0518	-75.56540734	-0.1838	-75.41123668	-0.0089	-75.56536303
4.378		-75.41490105	0.1909	-75.41129676	-0.0466	-75.56538303	-0.1686	-75.41123099	-0.0054	-75.56533948
4.428		-75.41491723	0.1807	-75.41128933	-0.0419	-75.56536104	-0.1548	-75.41122612	-0.0023	-75.56531832
4.478		-75.41493242	0.1712	-75.41128269	-0.0378	-75.56534112	-0.1423	-75.41122196	0.0003	-75.56529928
4.528		-75.41494669	0.1623	-75.41127675	-0.0340	-75.56532307	-0.1309	-75.41121842	0.0025	-75.56528215
4.578		-75.41496011	0.1538	-75.41127144	-0.0307	-75.56530668	-0.1207	-75.41121542	0.0044	-75.56526671
4.628		-75.41497273	0.1459	-75.41126669	-0.0277	-75.56529180	-0.1113	-75.41121290	0.0060	-75.56525281
4.678		-75.41498462	0.1385	-75.41126244	-0.0251	-75.56527828	-0.1028	-75.41121080	0.0073	-75.56524028
4.728		-75.41499581	0.1314	-75.41125864	-0.0227	-75.56526598	-0.0951	-75.41120908	0.0084	-75.56522898
4.828		-75.41501629	0.1186	-75.41125221	-0.0186	-75.56524458	-0.0817	-75.41120657	0.0100	-75.56520961
4.928		-75.41503450	0.1072	-75.41124709	-0.0154	-75.56522680	-0.0705	-75.41120509	0.0109	-75.56519386
5.028		-75.41505071	0.0970	-75.41124302	-0.0129	-75.56521198	-0.0612	-75.41120441	0.0113	-75.56518106
5.128		-75.41506516	0.0879	-75.41123979	-0.0108	-75.56519958	-0.0535	-75.41120434	0.0114	-75.56517064
5.228		-75.41507804	0.0798	-75.41123722	-0.0092	-75.56518900	-0.0468	-75.41120470	0.0111	-75.56516192
5.328		-75.41508955	0.0726	-75.41123519	-0.0080	-75.56518022	-0.0413	-75.41120537	0.0107	-75.56515500
5.428		-75.41509984	0.0662	-75.41123356	-0.0069	-75.56517255	-0.0365	-75.41120624	0.0102	-75.56514929
5.528		-75.41510905	0.0604	-75.41123225	-0.0061	-75.56516620	-0.0325	-75.41120721	0.0096	-75.56514459
5.628		-75.41511730	0.0552	-75.41123118	-0.0054	-75.56516075	-0.0291	-75.41120823	0.0089	-75.56514067
5.728		-75.41512471	0.0506	-75.41123029	-0.0049	-75.56515602	-0.0261	-75.41120925	0.0083	-75.56513737
5.828		-75.41513138	0.0464	-75.41122953	-0.0044	-75.56515189	-0.0235	-75.41121023	0.0077	-75.56513458
5.928		-75.41513738	0.0426	-75.41122888	-0.0040	-75.56514827	-0.0213	-75.41121115	0.0071	-75.56513218
6.028		-75.41514280	0.0392	-75.41122830	-0.0036	-75.56514508	-0.0193	-75.41121200	0.0066	-75.56513013
6.128		-75.41514769	0.0361	-75.41122779	-0.0033	-75.56514224	-0.0175	-75.41121278	0.0061	-75.56512833
6.228		-75.41515213	0.0333	-75.41122733	-0.0030	-75.56513972	-0.0159	-75.41121348	0.0056	-75.56512675

6.328		-75.41515615	0.0308	-75.41122691	-0.0028	-75.56513743	-0.0145	-75.41121412	0.0052	-75.56512534
6.428		-75.41515980	0.0285	-75.41122652	-0.0025	-75.56513541	-0.0132	-75.41121469	0.0049	-75.56512411
6.528		-75.41516313	0.0264	-75.41122616	-0.0023	-75.56513359	-0.0120	-75.41121520	0.0046	-75.56512302
6.628		-75.41516617	0.0245	-75.41122583	-0.0021	-75.56513194	-0.0110	-75.41121566	0.0043	-75.56512204
6.728		-75.41516895	0.0228	-75.41122552	-0.0019	-75.56513046	-0.0101	-75.41121608	0.0040	-75.56512117
6.828		-75.41517149	0.0212	-75.41122524	-0.0017	-75.56512913	-0.0092	-75.41121646	0.0038	-75.56512039
6.928		-75.41517382	0.0197	-75.41122498	-0.0016	-75.56512776	-0.0084	-75.41121680	0.0036	-75.56511969
7.028		-75.41517595	0.0184	-75.41122474	-0.0014	-75.56512667	-0.0077	-75.41121711	0.0034	-75.56511907
7.128		-75.41517792	0.0172	-75.41122452	-0.0013	-75.56512568	-0.0071	-75.41121740	0.0032	-75.56511852
7.228		-75.41517973	0.0160	-75.41122432	-0.0011	-75.56512479	-0.0065	-75.41121767	0.0030	-75.56511802
7.328		-75.41518140	0.0150	-75.41122414	-0.0010	-75.56512398	-0.0060	-75.41121792	0.0028	-75.56511758
7.428		-75.41518294	0.0140	-75.41122397	-0.0009	-75.56512325	-0.0056	-75.41121815	0.0027	-75.56511719
7.528		-75.41518436	0.0131	-75.41122383	-0.0008	-75.56512258	-0.0051	-75.41121838	0.0026	-75.56511685
7.628		-75.41518568	0.0123	-75.41122369	-0.0007	-75.56512198	-0.0048	-75.41121858	0.0024	-75.56511654
7.728		-75.41518690	0.0115	-75.41122357	-0.0007	-75.56512143	-0.0044	-75.41121878	0.0023	-75.56511627
7.828		-75.41518804	0.0108	-75.41122347	-0.0006	-75.56512043	-0.0038	-75.41121897	0.0022	-75.56511600
7.928		-75.41518909	0.0102	-75.41122337	-0.0005	-75.56511998	-0.0035	-75.41121915	0.0021	-75.56511579
8.028		-75.41519006	0.0095	-75.41122329	-0.0005	-75.56511957	-0.0032	-75.41121932	0.0020	-75.56511561
8.128		-75.41519097	0.0090	-75.41122321	-0.0004	-75.56511920	-0.0030	-75.41121948	0.0019	-75.56511545
8.228		-75.41519181	0.0084	-75.41122314	-0.0004	-75.56511886	-0.0028	-75.41121963	0.0018	-75.56511530
8.328		-75.41519260	0.0080	-75.41122308	-0.0004	-75.56511856	-0.0026	-75.41121978	0.0017	-75.56511518
8.428		-75.41519333	0.0075	-75.41122303	-0.0003	-75.56511828	-0.0024	-75.41121992	0.0016	-75.56511507
8.528		-75.41519402	0.0071	-75.41122298	-0.0003	-75.56511802	-0.0023	-75.41122005	0.0015	-75.56511497
8.628		-75.41519466	0.0067	-75.41122294	-0.0003	-75.56511778	-0.0021	-75.41122018	0.0014	-75.56511489
8.728		-75.41519525	0.0063	-75.41122290	-0.0003	-75.56511757	-0.0020	-75.41122029	0.0014	-75.56511482
8.828		-75.41519581	0.0059	-75.41122287	-0.0002	-75.56511737	-0.0019	-75.41122041	0.0013	-75.56511475
8.928		-75.41519633	0.0056	-75.41122284	-0.0002	-75.56511719	-0.0018	-75.41122051	0.0012	-75.56511470
9.028		-75.41519682	0.0053	-75.41122281	-0.0002	-75.56511703	-0.0017	-75.41122061	0.0012	-75.56511465
9.128		-75.41519728	0.0050	-75.41122279	-0.0002	-75.56511688	-0.0016	-75.41122071	0.0011	-75.56511461
9.228		-75.41519771	0.0047	-75.41122277	-0.0002	-75.56511674	-0.0015	-75.41122080	0.0010	-75.56511457
9.328		-75.41519811	0.0045	-75.41122275	-0.0002	-75.56511661	-0.0014	-75.41122088	0.0010	-75.56511454
9.428		-75.41519849	0.0043	-75.41122273	-0.0001	-75.56511649	-0.0013	-75.41122096	0.0009	-75.56511452
9.528		-75.41519885	0.0040	-75.41122272	-0.0001	-75.56511638	-0.0012	-75.41122104	0.0009	-75.56511450
9.628		-75.41519918	0.0038	-75.41122270	-0.0001	-75.56511628	-0.0012	-75.41122111	0.0008	-75.56511448
9.728		-75.41519949	0.0036	-75.41122269	-0.0001	-75.56511619	-0.0011	-75.41122118	0.0008	-75.56511446
20.000		-75.41520527	0.0000	-75.41122250	0.0000	-75.56511440	0.0000	-75.41122246	0.0000	-75.56511436

	E(R=20.0) -75.41122227		E(R=20.0) -75.56511417		DCE(R=20.0) -94.0694		Re 1.248		
					DCE		DCE (Re-shifted)		
ΔE2(vCASC1)	ΔE3(vCAS)	ΔE3(vCAS)	E3(vCASC1)	ΔE3(vCASC1)	vCASC11-SCGV B	Δ(vCASC11-SCGV B)	ΔR	vCASC11-SCGV B	Δ(vCASC11-SCGV B)
167.8758	-75.02170895	244.4233	-75.21985577	216.6530	-123.7924	-29.7230	-0.330	-123.7924	-29.7230
151.0069	-75.05662965	222.5103	-75.25410479	195.1614	-123.7600	-29.6906	-0.320	-123.7600	-29.6906
135.0784	-75.08964905	201.7903	-75.28645971	174.8583	-123.7389	-29.6695	-0.310	-123.7389	-29.6695
120.0309	-75.12086230	182.2037	-75.31701521	155.6845	-123.7284	-29.6590	-0.300	-123.7284	-29.6590
105.8079	-75.15035941	163.6939	-75.34586113	137.5834	-123.7279	-29.6585	-0.290	-123.7279	-29.6585
92.3566	-75.17822546	146.2077	-75.37308272	120.5016	-123.7369	-29.6675	-0.280	-123.7369	-29.6675
79.6275	-75.20454083	129.6946	-75.39876090	104.3883	-123.7546	-29.6852	-0.270	-123.7546	-29.6852
67.5753	-75.22938145	114.1069	-75.42297247	89.1953	-123.7805	-29.7111	-0.260	-123.7805	-29.7111
56.1585	-75.25281909	99.3995	-75.44579036	74.8768	-123.8139	-29.7445	-0.250	-123.8139	-29.7445
45.3401	-75.27492169	85.5299	-75.46728385	61.3895	-123.8543	-29.7849	-0.240	-123.8543	-29.7849
35.0870	-75.29575363	72.4577	-75.48751873	48.6919	-123.9010	-29.8316	-0.230	-123.9010	-29.8316
25.3701	-75.31537610	60.1444	-75.50655758	36.7448	-123.9534	-29.8840	-0.220	-123.9534	-29.8840
16.1637	-75.33384735	48.5535	-75.52445988	25.5110	-124.0111	-29.9416	-0.210	-124.0111	-29.9416
7.4451	-75.35122301	37.6501	-75.54128225	14.9548	-124.0733	-30.0039	-0.200	-124.0733	-30.0039
-0.8058	-75.36755624	27.4009	-75.55707854	5.0424	-124.1396	-30.0702	-0.190	-124.1396	-30.0702
-8.6072	-75.38289791	17.7738	-75.57190003	-4.2582	-124.2095	-30.1400	-0.180	-124.2095	-30.1400
-22.9274	-75.41079939	0.2654	-75.59881141	-21.1453	-124.3578	-30.2884	-0.160	-124.3578	-30.2884
-35.9342	-75.43529256	-15.1043	-75.62190701	-35.6381	-124.5143	-30.4449	-0.140	-124.5143	-30.4449
-48.8314	-75.45671099	-28.5446	-75.63977805	-46.8523	-124.6753	-30.6059	-0.120	-124.6753	-30.6059
-60.0234	-75.47535830	-40.2460	-75.65543840	-56.6793	-124.8373	-30.7679	-0.100	-124.8373	-30.7679
-69.6793	-75.49151002	-50.3813	-75.66905690	-65.2251	-124.9970	-30.9276	-0.080	-124.9970	-30.9276
-77.9524	-75.50541563	-59.1072	-75.68079716	-72.5922	-125.1513	-31.0819	-0.060	-125.1513	-31.0819
-84.9811	-75.51623843	-65.8986	-75.69081642	-78.8794	-125.2975	-31.2281	-0.040	-125.2975	-31.2281
-90.8911	-75.52518887	-71.5151	-75.69926427	-84.1805	-125.4331	-31.3637	-0.020	-125.4331	-31.3637
-95.7961	-75.53268765	-76.2207	-75.70628168	-88.5840	-125.5560	-31.4866	0.000	-125.5560	-31.4866
-99.7993	-75.53886977	-80.1000	-75.71200055	-92.1726	-125.6645	-31.5951	0.020	-125.6645	-31.5951
-102.9940	-75.54386062	-80.1000	-75.71654332	-95.0232	-125.7572	-31.6878	0.040	-125.7572	-31.6878
-105.4650	-75.54777606	-83.2318	-75.72002305	-97.2068	-125.8332	-31.7638	0.060	-125.8332	-31.7638
-107.2892	-75.55072278	-85.6888	-75.72254357	-98.7885	-125.8921	-31.8227	0.080	-125.8921	-31.8227
-108.5361	-75.55279870	-87.5379	-75.72419973	-99.8277	-125.9342	-31.8648	0.100	-125.9342	-31.8648
-109.2689	-75.55409339	-88.8406	-75.72507770	-100.3787	-125.9602	-31.8908	0.120	-125.9602	-31.8908
-109.5449	-75.55468855	-89.6530	-75.72525515	-100.4900	-125.9718	-31.9024	0.140	-125.9718	-31.9024
-109.4160	-75.55465847	-90.0265	-75.72480154	-100.2054	-125.9717	-31.9023	0.160	-125.9717	-31.9023
-108.9292	-75.55407047	-90.0076	-75.72377821	-99.5632	-125.9638	-31.8944	0.180	-125.9638	-31.8944
-108.1272	-75.55298518	-89.6386	-75.72223830	-98.5969	-125.9534	-31.8840	0.200	-125.9534	-31.8840
-107.0485	-75.55145693	-88.9576	-75.72022669	-97.3346	-125.9480	-31.8786	0.220	-125.9480	-31.8786
-105.7281	-75.54953381	-87.9986	-75.71777973	-95.7991	-125.9570	-31.8876	0.240	-125.9570	-31.8876
-104.1975	-75.54725778	-86.7918	-75.71492525	-94.0079	-125.9926	-31.9232	0.260	-125.9926	-31.9232
-102.4853	-75.54466445	-85.3636	-75.71168310	-91.9734	-126.0694	-32.0000	0.280	-126.0694	-32.0000
-100.6173	-75.54178265	-83.7362	-75.70806714	-89.7044	-126.2034	-32.1340	0.300	-126.2034	-32.1340
-98.6166	-75.53863373	-81.9279	-75.70408969	-87.2085	-126.4093	-32.3399	0.320	-126.4093	-32.3399
-96.5043	-75.53523065	-79.9519	-75.69976861	-84.4970	-126.6965	-32.6271	0.340	-126.6965	-32.6271
-93.2863	-75.53157726	-77.8164	-75.69513485	-81.5892	-128.0770	-34.0075	0.360	-128.0770	-34.0075
-90.1962	-75.52766911	-75.5239	-75.69023640	-78.5154	-129.3212	-35.2518	0.380	-129.3212	-35.2518
-87.2317	-75.52349814	-73.0715	-75.68513519	-75.3143	-130.4232	-36.3537	0.400	-130.4232	-36.3537
-84.3750	-75.51906333	-70.4542	-75.67989885	-72.0285	-131.3862	-37.3168	0.420	-131.3862	-37.3168
-81.6071	-75.51438458	-67.6713	-75.67459211	-68.6985	-132.2139	-38.1445	0.440	-132.2139	-38.1445
-78.9117	-75.50950970	-64.7353	-75.66927151	-65.3597	-132.9096	-38.8402	0.460	-132.9096	-38.8402
-76.2767	-75.50450677	-61.6763	-75.66398363	-62.0415	-133.4771	-39.4077	0.480	-133.4771	-39.4077
-73.6936	-75.49944809	-58.5369	-75.65876568	-58.7672	-133.9201	-39.8507	0.500	-133.9201	-39.8507
-71.1572	-75.49439765	-55.3625	-75.65364685	-55.5551	-134.2424	-40.1730	0.520	-134.2424	-40.1730
-68.6646	-75.48940647	-52.1933	-75.64864994	-52.4195	-134.4482	-40.3788	0.540	-134.4482	-40.3788
-66.2146	-75.48451330	-49.0613	-75.64379265	-49.3715	-134.5418	-40.4724	0.560	-134.5418	-40.4724
-63.8069	-75.47974704	-45.9908	-75.63908870	-46.4197	-134.5276	-40.4582	0.580	-134.5276	-40.4582
-61.4419	-75.47512920	-43.0000	-75.63454867	-43.5708	-134.4106	-40.3412	0.600	-134.4106	-40.3412
-59.1207	-75.47067584	-40.1022	-75.63018045	-40.8297	-134.1957	-40.1263	0.620	-134.1957	-40.1263
-56.8443	-75.46639894	-37.3077	-75.62598989	-38.2001	-133.8882	-39.8187	0.640	-133.8882	-39.8187
-54.6140	-75.46230729	-34.6239	-75.62198095	-35.6845	-133.4936	-39.4242	0.660	-133.4936	-39.4242
-52.4310	-75.45840715	-32.0563	-75.61815604	-33.2843	-133.0178	-38.9484	0.680	-133.0178	-38.9484
-50.2965	-75.45470262	-29.6090	-75.61451620	-31.0002	-132.4666	-38.3971	0.700	-132.4666	-38.3971
-48.2118	-75.45119596	-27.2843	-75.61106128	-28.8323	-131.8460	-37.7766	0.720	-131.8460	-37.7766
-46.1778	-75.44788777	-25.0839	-75.60779000	-26.7795	-131.1622	-37.0928	0.740	-131.1622	-37.0928
-44.1956	-75.44447716	-23.0080	-75.60470004	-24.8405	-130.4213	-36.3519	0.760	-130.4213	-36.3519
-42.2660	-75.44186183	-21.0560	-75.60178826	-23.0133	-129.6294	-35.5600	0.780	-129.6294	-35.5600
-40.3896	-75.43913826	-19.2266	-75.59905071	-21.2955	-128.7924	-34.7230	0.800	-128.7924	-34.7230

-38.5673	-75.43660173	-17.5176	-75.59648265	-19.6840	-127.9163	-33.8469	0.820	-127.9163	-33.8469
-36.7994	-75.43424653	-15.9259	-75.59407876	-18.1756	-127.0067	-32.9373	0.840	-127.0067	-32.9373
-35.0863	-75.43206604	-14.4479	-75.59183318	-16.7664	-126.0692	-31.9997	0.860	-126.0692	-31.9997
-33.4284	-75.43005288	-13.0797	-75.58973958	-15.4527	-125.1091	-31.0397	0.880	-125.1091	-31.0397
-31.8258	-75.42819910	-11.8164	-75.58779129	-14.2301	-124.1317	-30.0623	0.900	-124.1317	-30.0623
-30.2784	-75.42649626	-10.6531	-75.58598140	-13.0944	-123.1420	-29.0726	0.920	-123.1420	-29.0726
-28.7864	-75.42493563	-9.5846	-75.58430269	-12.0410	-122.1448	-28.0754	0.940	-122.1448	-28.0754
-27.3493	-75.42350833	-8.6053	-75.58274799	-11.0654	-121.1448	-27.0754	0.960	-121.1448	-27.0754
-25.9671	-75.42220545	-7.7096	-75.58131009	-10.1631	-120.1462	-26.0768	0.980	-120.1462	-26.0768
-22.7478	-75.41943527	-6.8921	-75.57817948	-8.1986	-117.6826	-23.6132	1.030	-117.6826	-23.6132
-19.8582	-75.41725767	-5.1537	-75.57562672	-6.5967	-115.3088	-21.2394	1.080	-115.3088	-21.2394
-17.2843	-75.41555654	-3.7873	-75.57355369	-5.2959	-113.0668	-18.9974	1.130	-113.0668	-18.9974
-15.0089	-75.41423340	-2.7198	-75.57187410	-4.2419	-110.9852	-16.9158	1.180	-110.9852	-16.9158
-13.0113	-75.41320762	-1.8895	-75.57051451	-3.3888	-109.0802	-15.0108	1.230	-109.0802	-15.0108
-11.2686	-75.41241474	-1.2458	-75.56941377	-2.6980	-107.3575	-13.2881	1.280	-107.3575	-13.2881
-9.7567	-75.41180404	-0.7483	-75.56852182	-2.1383	-105.8145	-11.7451	1.330	-105.8145	-11.7451
-8.4507	-75.41133589	-0.3651	-75.56779814	-1.6842	-104.4427	-10.3733	1.380	-104.4427	-10.3733
-7.3263	-75.41097947	-0.0713	-75.56721016	-1.3153	-103.2299	-9.1605	1.430	-103.2299	-9.1605
-6.3604	-75.41071071	0.1524	-75.56673182	-1.0151	-102.1619	-8.0925	1.480	-102.1619	-8.0925
-5.5315	-75.41051083	0.3210	-75.56634228	-0.7707	-101.2239	-7.1545	1.530	-101.2239	-7.1545
-4.8205	-75.41036510	0.4464	-75.56602484	-0.5715	-100.4016	-6.3322	1.580	-100.4016	-6.3322
-4.2101	-75.41026190	0.5379	-75.56576612	-0.4091	-99.6817	-5.6123	1.630	-99.6817	-5.6123
-3.6856	-75.41019209	0.6026	-75.56555537	-0.2769	-99.0519	-4.9824	1.680	-99.0519	-4.9824
-3.2340	-75.41014841	0.6464	-75.56538391	-0.1693	-98.5010	-4.4316	1.730	-98.5010	-4.4316
-2.8444	-75.41012511	0.6739	-75.56524472	-0.0819	-98.0191	-3.9497	1.780	-98.0191	-3.9497
-2.5075	-75.41011762	0.6885	-75.56513208	-0.0112	-97.5970	-3.5276	1.830	-97.5970	-3.5276
-2.2153	-75.41012231	0.6932	-75.56504133	0.0457	-97.2266	-3.1572	1.880	-97.2266	-3.1572
-1.9614	-75.41013631	0.6902	-75.56496867	0.0913	-96.9009	-2.8315	1.930	-96.9009	-2.8315
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-1.5465	-75.41018351	0.6683	-75.56486563	0.1560	-96.3602	-2.2908	2.030	-96.3602	-2.2908
-1.3771	-75.41021345	0.6518	-75.56483056	0.1780	-96.1356	-2.0662	2.080	-96.1356	-2.0662
-1.2282	-75.41024600	0.6330	-75.56480399	0.1946	-95.9363	-1.8669	2.130	-95.9363	-1.8669
-1.0937	-75.41028025	0.6126	-75.56478442	0.2069	-95.7626	-1.6932	2.180	-95.7626	-1.6932
-0.9729	-75.41031550	0.5911	-75.56477067	0.2155	-95.6099	-1.5405	2.230	-95.6099	-1.5405
-0.8664	-75.41035120	0.5690	-75.56476173	0.2212	-95.4732	-1.4038	2.280	-95.4732	-1.4038
-0.7725	-75.41038691	0.5466	-75.56475672	0.2243	-95.3506	-1.2812	2.330	-95.3506	-1.2812
-0.6896	-75.41042230	0.5242	-75.56475495	0.2254	-95.2406	-1.1711	2.380	-95.2406	-1.1711
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-0.5511	-75.41049118	0.4801	-75.56475882	0.2230	-95.0523	-0.9829	2.480	-95.0523	-0.9829
-0.4935	-75.41052433	0.4588	-75.56476356	0.2200	-94.9718	-0.9024	2.530	-94.9718	-0.9024
-0.4423	-75.41055646	0.4380	-75.56476966	0.2162	-94.8991	-0.8297	2.580	-94.8991	-0.8297
-0.3969	-75.41058750	0.4178	-75.56477685	0.2117	-94.8334	-0.7640	2.630	-94.8334	-0.7640
-0.3564	-75.41061741	0.3983	-75.56478487	0.2066	-94.7738	-0.7044	2.680	-94.7738	-0.7044
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-0.2883	-75.41067369	0.3615	-75.56480261	0.1955	-94.6707	-0.6013	2.780	-94.6707	-0.6013
-0.2597	-75.41070005	0.3442	-75.56481201	0.1896	-94.6261	-0.5566	2.830	-94.6261	-0.5566
-0.2342	-75.41072525	0.3277	-75.56482160	0.1836	-94.5854	-0.5160	2.880	-94.5854	-0.5160
-0.2113	-75.41074928	0.3119	-75.56483128	0.1775	-94.5483	-0.4789	2.930	-94.5483	-0.4789
-0.1908	-75.41077218	0.2968	-75.56484097	0.1714	-94.5144	-0.4450	2.980	-94.5144	-0.4450
-0.1725	-75.41079399	0.2824	-75.56485060	0.1654	-94.4834	-0.4140	3.030	-94.4834	-0.4140
-0.1560	-75.41081472	0.2687	-75.56486011	0.1594	-94.4550	-0.3855	3.080	-94.4550	-0.3855
-0.1413	-75.41083443	0.2557	-75.56486947	0.1536	-94.4289	-0.3595	3.130	-94.4289	-0.3595
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-0.1160	-75.41087092	0.2316	-75.56488759	0.1422	-94.3829	-0.3135	3.230	-94.3829	-0.3135
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-0.0956	-75.41090378	0.2099	-75.56490479	0.1314	-94.3439	-0.2745	3.330	-94.3439	-0.2745
-0.0869	-75.41091895	0.1999	-75.56491301	0.1262	-94.3267	-0.2572	3.380	-94.3267	-0.2572
-0.0790	-75.41093335	0.1903	-75.56492096	0.1212	-94.3107	-0.2413	3.430	-94.3107	-0.2413
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-0.0598	-75.41097224	0.1727	-75.56494323	0.1073	-94.2697	-0.2003	3.580	-94.2697	-0.2003
-0.0499	-75.41099495	0.1569	-75.56495675	0.0988	-94.2471	-0.1777	3.680	-94.2471	-0.1777
-0.0419	-75.41101540	0.1426	-75.56496927	0.0909	-94.2276	-0.1582	3.780	-94.2276	-0.1582
-0.0353	-75.41103383	0.1298	-75.56498081	0.0837	-94.2108	-0.1414	3.880	-94.2108	-0.1414
-0.0298	-75.41105045	0.1182	-75.56499134	0.0771	-94.1961	-0.1267	3.980	-94.1961	-0.1267
-0.0255	-75.41106544	0.1078	-75.56500110	0.0710	-94.1833	-0.1139	4.080	-94.1833	-0.1139
-0.0219	-75.41107897	0.0984	-75.56500955	0.0657	-94.1721	-0.1026	4.180	-94.1721	-0.1026
-0.0190	-75.41109118	0.0899	-75.56501784	0.0604	-94.1623	-0.0929	4.280	-94.1623	-0.0929
-0.0165	-75.41110222	0.0823	-75.56502540	0.0557	-94.1537	-0.0843	4.380	-94.1537	-0.0843
-0.0144	-75.41111219	0.0753	-75.56503231	0.0514	-94.1461	-0.0767	4.480	-94.1461	-0.0767
-0.0127	-75.41112120	0.0691	-75.56503861	0.0474	-94.1393	-0.0699	4.580	-94.1393	-0.0699
-0.0112	-75.41112936	0.0634	-75.56504437	0.0438	-94.1333	-0.0639	4.680	-94.1333	-0.0639
-0.0099	-75.41113675	0.0583	-75.56504963	0.0405	-94.1279	-0.0585	4.780	-94.1279	-0.0585
-0.0088	-75.41114345	0.0537	-75.56505443	0.0375	-94.1230	-0.0536	4.880	-94.1230	-0.0536
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-0.0069	-75.41115504	0.0457	-75.56506280	0.0322	-94.1147	-0.0453	5.080	-94.1147	-0.0453
-0.0061	-75.41116006	0.0422	-75.56506650	0.0299	-94.1111	-0.0417	5.180	-94.1111	-0.0417
-0.0054	-75.41116463	0.0390	-75.56506988	0.0278	-94.1079	-0.0385	5.280	-94.1079	-0.0385
-0.0048	-75.41116880	0.0362	-75.56507294	0.0259	-94.1050	-0.0355	5.380	-94.1050	-0.0355
-0.0043	-75.41117261	0.0336	-75.56507580	0.0241	-94.1023	-0.0329	5.480	-94.1023	-0.0329
-0.0038	-75.41117609	0.0312	-75.56507843	0.0224	-94.0999	-0.0304	5.580	-94.0999	-0.0304
-0.0033	-75.41117928	0.0290	-75.56508050	0.0211	-94.0975	-0.0281	5.680	-94.0975	-0.0281
-0.0030	-75.41118220	0.0270	-75.56508274	0.0197	-94.0955	-0.0261	5.780	-94.0955	-0.0261
-0.0026	-75.41118488	0.0251	-75.56508480	0.0184	-94.0937	-0.0242	5.880	-94.0937	-0.0242
-0.0023	-75.41118735	0.0235	-75.56508672	0.0172	-94.0920	-0.0225	5.980	-94.0920	-0.0225
-0.0020	-75.41118963	0.0219	-75.56508849	0.0161	-94.0904	-0.0210	6.080	-94.0904	-0.0210
-0.0018	-75.41119173	0.0205	-75.56509013	0.0151	-94.0890	-0.0196	6.180	-94.0890	-0.0196
-0.0016	-75.41119366	0.0192	-75.56509166	0.0141	-94.0877	-0.0183	6.280	-94.0877	-0.0183
-0.0014	-75.41119546	0.0180	-75.56509307	0.0132	-94.0865	-0.0170	6.380	-94.0865	-0.0170
-0.0012	-75.41119712	0.0168	-75.56509439	0.0124	-94.0854	-0.0159	6.480	-94.0854	-0.0159
-0.0010	-75.41119866	0.0158	-75.56509420	0.0125	-94.0840	-0.0146	6.580	-94.0840	-0.0146
-0.0009	-75.41120009	0.0148	-75.56509535	0.0118	-94.0831	-0.0137	6.680	-94.0831	-0.0137
-0.0008	-75.41120141	0.0139	-75.56509643	0.0111	-94.0822	-0.0128	6.780	-94.0822	-0.0128
-0.0007	-75.41120265	0.0131	-75.56509744	0.0105	-94.0814	-0.0120	6.880	-94.0814	-0.0120
-0.0006	-75.41120380	0.0123	-75.56509838	0.0099	-94.0807	-0.0112	6.980	-94.0807	-0.0112
-0.0005	-75.41120487	0.0116	-75.56509926	0.0094	-94.0800	-0.0106	7.080	-94.0800	-0.0106
-0.0004	-75.41120587	0.0109	-75.56510009	0.0088	-94.0793	-0.0099	7.180	-94.0793	-0.0099
-0.0004	-75.41120680	0.0103	-75.56510086	0.0084	-94.0787	-0.0093	7.280	-94.0787	-0.0093
-0.0003	-75.41120767	0.0097	-75.56510159	0.0079	-94.0782	-0.0088	7.380	-94.0782	-0.0088
-0.0003	-75.41120849	0.0092	-75.56510227	0.0075	-94.0777	-0.0083	7.480	-94.0777	-0.0083
-0.0002	-75.41120925	0.0086	-75.56510291	0.0071	-94.0772	-0.0078	7.580	-94.0772	-0.0078
-0.0002	-75.41120996	0.0082	-75.56510351	0.0067	-94.0768	-0.0074	7.680	-94.0768	-0.0074
-0.0002	-75.41121063	0.0077	-75.56510407	0.0063	-94.0764	-0.0070	7.780	-94.0764	-0.0070
-0.0002	-75.41121126	0.0073	-75.56510460	0.0060	-94.0760	-0.0066	7.880	-94.0760	-0.0066
-0.0001	-75.41121185	0.0069	-75.56510510	0.0057	-94.0756	-0.0062	7.980	-94.0756	-0.0062
-0.0001	-75.41121240	0.0065	-75.56510557	0.0054	-94.0753	-0.0059	8.080	-94.0753	-0.0059
-0.0001	-75.41121292	0.0062	-75.56510602	0.0051	-94.0750	-0.0056	8.180	-94.0750	-0.0056
-0.0001	-75.41121340	0.0059	-75.56510643	0.0049	-94.0747	-0.0053	8.280	-94.0747	-0.0053
-0.0001	-75.41121386	0.0056	-75.56510683	0.0046	-94.0744	-0.0050	8.380	-94.0744	-0.0050
-0.0001	-75.41121429	0.0053	-75.56510720	0.0044	-94.0742	-0.0048	8.480	-94.0742	-0.0048
0.0000	-75.41122227	0.0050	-75.56511417	0.0000	-94.0694	0.0000	18.752	-94.0694	0.0000

N2: RHF, CCSD(T), SCGVB, vCAS and vCASCI ENERGIES

R(Å)	E(R=∞)		E(R=∞)		E(R=20.0)		E(R=20.0)		E(R=20.0)		EDCE(R=20.0)		
	-108.80045046		-109.05019088		-108.80044983		-108.80044983		-109.03368898		-146.3598		
					SCGVB		vCAS3: (occ,3,1,1,0,3,1,1,0;closed,2,0,0,0,2,0,0,0) + (occ,3,1,1,0,3,1,1,0;closed,1,0,0,0,1,0,0,0);frozen DCE						
	E(RHF)	ΔE(RHD)	E[CCSD(T)]	ΔE[CCSD(T)]	E(SCGVB)	ΔE(SCGVB)	E(vCAS1)	E(vCAS3)	ΔE(vCAS3)	E(vCASCI3)	ΔE(vCASCI3)	vCASCI3-SCGVB	Δ(vCASCI3-SCGVB)
0.771					-108.39450127	254.7366	-108.43301877	-108.44125791	225.3964	-108.70331656	207.3119	-193.7846	-47.4248
0.781					-108.45431664	217.2019	-108.49334090	-108.50170944	187.4625	-108.76337041	169.6275	-193.9342	-47.5744
0.791					-108.50990047	182.3225	-108.54943475	-108.55793248	152.1820	-108.81920276	134.5922	-194.0902	-47.7304
0.801					-108.56150825	149.9381	-108.60155548	-108.61018215	119.3948	-108.87106854	102.0459	-194.2521	-47.8922
0.811					-108.60938014	119.8981	-108.64994286	-108.65869822	88.9505	-108.91920740	71.8383	-194.4196	-48.0598
0.821					-108.65374190	92.0606	-108.69482228	-108.70370602	60.7077	-108.96384458	43.8280	-194.5924	-48.2326
0.831					-108.69480581	66.2926	-108.73640559	-108.74541737	34.5334	-109.00519185	17.8822	-194.7702	-48.4104
0.841					-108.73277151	42.4688	-108.77489194	-108.78403141	10.3027	-109.04344832	-6.1241	-194.9527	-48.5929
0.851					-108.76782674	20.4713	-108.81046862	-108.81973539	-12.1019	-109.07880122	-28.3084	-195.1395	-48.7797
0.861					-108.80014812	0.1893	-108.84331175	-108.85270541	-32.7909	-109.11142663	-48.7811	-195.3303	-48.9704
0.871					-108.82990183	-18.4814	-108.87358699	-108.88310708	-51.8682	-109.14149021	-67.6463	-195.5247	-49.1649
0.881					-108.85724421	-35.6390	-108.90145019	-108.91109622	-69.4317	-109.16914777	-85.0017	-195.7225	-49.3627
0.891					-108.88232247	-51.3759	-108.92704796	-108.93681942	-85.5732	-109.19454593	-100.9393	-195.9232	-49.5634
0.901					-108.90527513	-65.7789	-108.95051830	-108.96041463	-100.3794	-109.21782266	-115.5457	-196.1266	-49.7668
0.911					-108.92623263	-78.9299	-108.97199106	-108.98201167	-113.9318	-109.23910783	-128.9023	-196.3322	-49.9724
0.921					-108.94531782	-90.9061	-108.99158849	-109.00173274	-126.3070	-109.25852368	-141.0859	-196.5397	-50.1799
0.941					-108.97832726	-111.6198	-109.02561090	-109.03600040	-147.8102	-109.29220097	-162.2188	-196.9588	-50.5990
0.961					-109.00515086	-128.4519	-109.05342789	-109.06405958	-165.4176	-109.31969693	-179.4727	-197.3807	-51.0209
0.981					-109.02654110	-141.8744	-109.07578661	-109.08665705	-179.5978	-109.34175873	-193.3167	-197.8021	-51.4423
1.001					-109.04316658	-152.3071	-109.09335014	-109.10445547	-190.7665	-109.35904949	-204.1668	-198.2196	-51.8598
1.021	-108.98717226	-117.1697	-109.38704689	-211.3804	-109.05562184	-160.1229	-109.10670723	-109.11804309	-199.2928	-109.37215795	-212.3925	-198.6294	-52.2696
1.041	-108.99267705	-120.6240	-109.39649106	-217.3067	-109.06443587	-165.6538	-109.11638087	-109.12794240	-205.5047	-109.38160702	-218.3219	-199.0279	-52.6681
1.061	-108.99485748	-121.9923	-109.40273788	-221.2266	-109.07007967	-169.1953	-109.12283587	-109.13461763	-209.6935	-109.38786135	-222.2466	-199.4111	-53.0512
1.081	-108.99412697	-121.5339	-109.40619957	-223.3989	-109.07297284	-171.0108	-109.12648547	-109.13848138	-212.1180	-109.39133388	-224.4256	-199.7746	-53.4148
1.101	-108.99085328	-119.4796	-109.40724249	-224.0533	-109.07348944	-171.3350	-109.12769716	-109.13990051	-213.0086	-109.39239170	-225.0894	-200.1142	-53.7544
1.121	-108.98536363	-116.0348	-109.40619228	-223.3943	-109.07196305	-170.3772	-109.12679789	-109.13920121	-212.5697	-109.39136117	-224.4427	-200.4254	-54.0656
1.141	-108.9794925	-111.3822	-109.40333831	-221.6034	-109.06869132	-168.3241	-109.12407853	-109.13667358	-210.9836	-109.38853240	-222.6677	-200.7033	-54.3435
1.161	-108.96886937	-105.6845	-109.39893769	-218.8420	-109.06393987	-165.3425	-109.11979789	-109.13257561	-208.4121	-109.38416328	-219.9260	-200.9433	-54.5835
1.181	-108.95835471	-99.0864	-109.39321881	-215.2533	-109.05794576	-161.5812	-109.11418622	-109.12713668	-204.9991	-109.37848295	-216.3615	-201.1402	-54.7804
1.201					-109.05092057	-157.1728	-109.10744837	-109.12056071	-200.8727	-109.37169491	-212.1020	-201.2890	-54.9292
1.221					-109.04305306	-152.2359	-109.09976649	-109.11302887	-196.1463	-109.36397985	-207.2607	-201.3846	-55.0248
1.241					-109.03451155	-146.8760	-109.09130246	-109.10470205	-190.9212	-109.35549788	-201.9382	-201.4220	-55.0622
1.261					-109.02544594	-141.1872	-109.08220009	-109.09572299	-185.2867	-109.34639095	-196.2235	-201.3961	-55.0363
1.281					-109.01598958	-135.2533	-109.07258705	-109.08621826	-179.3224	-109.33678459	-190.1954	-201.3019	-54.9421
1.301					-109.00626088	-129.1484	-109.06257651	-109.07629992	-173.0986	-109.32678974	-183.9235	-201.1349	-54.7751
1.321					-108.99636468	-122.9384	-109.05226877	-109.06606712	-166.6774	-109.31650422	-177.4693	-200.8906	-54.5308
1.341					-108.98639353	-116.6815	-109.04175259	-109.05560743	-160.1138	-109.30601416	-170.8867	-200.5650	-54.2052
1.361					-108.97642881	-110.4285	-109.03110643	-109.04499812	-153.4564	-109.29539524	-164.2232	-200.1545	-53.7947
1.381					-108.96654163	-104.2242	-109.02039957	-109.03430729	-146.7478	-109.28471384	-157.5205	-199.6561	-53.2963
1.401					-108.95679379	-98.1073	-109.00969315	-109.02359487	-140.0257	-109.27402800	-150.8150	-199.0675	-52.7077
1.421					-108.94723848	-92.1113	-108.99904105	-109.01291354	-133.3230	-109.26338841	-144.1386	-198.3871	-52.0273
1.441					-108.93792098	-86.2645	-108.98849071	-109.00230961	-126.6689	-109.25283921	-137.5189	-197.6142	-51.2544
1.461					-108.92887931	-80.5907	-108.97808391	-108.99182371	-120.0889	-109.24241877	-130.9799	-196.7490	-50.3892
1.481					-108.92014477	-75.1097	-108.96785741	-108.98149157	-113.6054	-109.23216035	-124.5427	-195.7928	-49.4330
1.501					-108.91174248	-69.8372	-108.95784353	-108.97134454	-107.2381	-109.22209271	-118.2251	-194.7477	-48.3879
1.521					-108.90369190	-64.7854	-108.94807071	-108.96141023	-101.0042	-109.21224069	-112.0429	-193.6173	-47.2575
1.541					-108.89600724	-59.9632	-108.93856391	-108.95171295	-94.9191	-109.20262566	-106.0094	-192.4060	-46.0462
1.561					-108.88869800	-55.3766	-108.92934506	-108.94227415	-88.9961	-109.19326597	-100.1361	-191.1193	-44.7595
1.581					-108.88176939	-51.0288	-108.92043331	-108.93311282	-83.2473	-109.18417732	-94.4329	-189.7639	-43.4041
1.601					-108.87522279	-46.9208	-108.91184532	-108.92424577	-77.6831	-109.17537303	-88.9081	-188.3472	-41.9874
1.621					-108.86905618	-43.0511	-108.90359542	-108.91568785	-72.3130	-109.16686438	-83.5688	-186.8775	-40.5177
1.641					-108.86326463	-39.4169	-108.89569576	-108.90745221	-67.1450	-109.15866078	-78.4210	-185.3639	-39.0041
1.661					-108.85784067	-36.0133	-108.88815636	-108.89955033	-62.1865	-109.15076992	-73.4694	-183.8159	-37.4561
1.681					-108.85277478	-32.8344	-108.88098510	-108.89199214	-57.4437	-109.14319797	-68.7179	-182.2433	-35.8835
1.701					-108.84805570	-29.8731	-108.87418776	-108.88478598	-52.9217	-109.13594960	-64.1695	-180.6562	-34.2964
1.721					-108.84367085	-27.1216	-108.86776792	-108.87793855	-48.6249	-109.12902801	-59.8262	-179.0644	-32.7046
1.741					-108.83960663	-24.5713	-108.86172694	-108.87145481	-44.5563	-109.12243509	-55.6890	-177.4776	-31.1178
1.761					-108.83584874	-22.2132	-108.85606386	-108.86533781	-40.7178	-109.11617129	-51.7584	-175.9051	-29.5453
1.781					-108.83238239	-20.0380	-108.85077547	-108.85958858	-37.1101	-109.11023568	-48.0338	-174.3556	-27.9958
1.801					-108.82919254	-18.0363	-108.84585619	-108.85420599	-33.7325	-109.10462594	-44.5136	-172.8371	-26.4773
1.821					-108.82626406	-16.1987	-108.84129825	-108.84918661	-30.5828	-109.09933838	-41.1956	-171.3568	-24.9970
1.841					-108.82358190	-14.5156	-108.83709173	-108.84452467	-27.6574	-109.09436786	-38.0766	-169.9208	-23.5610
1.861					-108.82113118	-12.9777	-108.83322475	-108.84021209	-24.9512	-109.08970794	-35.1524	-168.5345	-22.1747
1.881					-108.81889728	-11.5760	-108.82968367	-108.83623855	-22.4578	-109.08535083	-32.4183	-167.2022	-20.8424
1.901					-108.81686594	-10.3013	-108.82645338	-108.83259170	-20.1693	-109.08128749	-29.8685	-165.9271	-19.5673

1.921	-108.81502329	-9.1450	-108.82351760	-108.82925738	-18.0770	-109.07750774	-27.4967	-164.7115	-18.3517
1.941	-108.81335591	-8.0987	-108.82085912	-108.82621994	-16.1710	-109.07400041	-25.2958	-163.5569	-17.1971
1.961	-108.81185088	-7.1543	-108.81846021	-108.82346259	-14.4407	-109.07075345	-23.2583	-162.4638	-16.1040
1.981	-108.81049577	-6.3039	-108.81630284	-108.82096775	-12.8752	-109.06775412	-21.3762	-161.4321	-15.0723
2.001	-108.80927871	-5.5402	-108.81436899	-108.81871740	-11.4631	-109.06498921	-19.6412	-160.4608	-14.1010
2.021	-108.80818840	-4.8560	-108.81264091	-108.81669343	-10.1930	-109.06244517	-18.0448	-159.5486	-13.1888
2.041	-108.80721410	-4.2446	-108.81110131	-108.81487793	-9.0538	-109.06010833	-16.5784	-158.6936	-12.3338
2.061	-108.80634567	-3.6997	-108.80973356	-108.81325343	-8.0344	-109.05796506	-15.2335	-157.8936	-11.5338
2.081	-108.80557358	-3.2152	-108.80852180	-108.81180309	-7.1243	-109.05600193	-14.0016	-157.1462	-10.7864
2.131	-108.80400762	-2.2325	-108.80607890	-108.80883641	-5.2627	-109.05179740	-11.3632	-155.4905	-9.1307
2.181	-108.80286598	-1.5162	-108.80431249	-108.80663661	-3.8823	-109.04844725	-9.2610	-154.1046	-7.7448
2.231	-108.80204730	-1.0024	-108.80305342	-108.80501893	-2.8672	-109.04578431	-7.5899	-152.9473	-6.5875
2.281	-108.80147036	-0.6404	-108.80216840	-108.80383652	-2.1252	-109.04366750	-6.2616	-151.9810	-5.6212
2.331	-108.80107155	-0.3901	-108.80155513	-108.80297582	-1.5851	-109.04198116	-5.2034	-151.1731	-4.8133
2.381	-108.80080198	-0.2210	-108.80113675	-108.80235077	-1.1929	-109.04063243	-4.3571	-150.4959	-4.1361
2.431	-108.80062476	-0.1098	-108.80085647	-108.80189712	-0.9082	-109.03954784	-3.6765	-149.9265	-3.5667
2.481	-108.80051245	-0.0393	-108.80067284	-108.80156747	-0.7013	-109.03866991	-3.1256	-149.4461	-3.0863
2.531	-108.80044495	0.0031	-108.80055600	-108.80132711	-0.5505	-109.03795399	-2.6763	-149.0392	-2.6794
2.581	-108.80040770	0.0264	-108.80048463	-108.80115086	-0.4399	-109.03736552	-2.3071	-148.6933	-2.3335
2.631	-108.80039034	0.0373	-108.80044364	-108.80102052	-0.3581	-109.03687781	-2.0010	-148.3982	-2.0384
2.681	-108.80038555	0.0403	-108.80042250	-108.80092299	-0.2969	-109.03647023	-1.7453	-148.1454	-1.7856
2.731	-108.80038832	0.0386	-108.80041394	-108.80084892	-0.2504	-109.03612685	-1.5298	-147.9282	-1.5684
2.781	-108.80039523	0.0343	-108.80041300	-108.80079168	-0.2145	-109.03583531	-1.3468	-147.7409	-1.3811
2.831	-108.80040406	0.0287	-108.80041639	-108.80074655	-0.1862	-109.03558600	-1.1904	-147.5789	-1.2191
2.881	-108.80041341	0.0229	-108.80042196	-108.80071023	-0.1634	-109.03537142	-1.0557	-147.4384	-1.0786
2.931	-108.80042244	0.0172	-108.80042838	-108.80068041	-0.1447	-109.03518562	-0.9392	-147.3161	-0.9563
2.981	-108.80043072	0.0120	-108.80043483	-108.80065548	-0.1290	-109.03502394	-0.8377	-147.2095	-0.8497
3.031	-108.80043803	0.0074	-108.80044089	-108.80063430	-0.1158	-109.03488262	-0.7490	-147.1162	-0.7564
3.081	-108.80044434	0.0034	-108.80044632	-108.80061607	-0.1043	-109.03475862	-0.6712	-147.0345	-0.6747
3.131	-108.80044967	0.0001	-108.80045105	-108.80060022	-0.0944	-109.03464947	-0.6027	-146.9626	-0.6028
3.181	-108.80045411	-0.0027	-108.80045506	-108.80058632	-0.0856	-109.03455309	-0.5422	-146.8994	-0.5396
3.231	-108.80045774	-0.0050	-108.80045840	-108.80057405	-0.0779	-109.03446778	-0.4887	-146.8435	-0.4837
3.281	-108.80046065	-0.0068	-108.80046111	-108.80056314	-0.0711	-109.03439207	-0.4412	-146.7942	-0.4344
3.331	-108.80046291	-0.0082	-108.80046323	-108.80055338	-0.0650	-109.03432472	-0.3989	-146.7505	-0.3907
3.381	-108.80046462	-0.0093	-108.80046484	-108.80054459	-0.0595	-109.03426467	-0.3613	-146.7118	-0.3520
3.431	-108.80046581	-0.0100	-108.80046597	-108.80053664	-0.0545	-109.03421100	-0.3276	-146.6774	-0.3175
3.481	-108.80046656	-0.0105	-108.80046667	-108.80052938	-0.0499	-109.03416294	-0.2974	-146.6467	-0.2869
3.531	-108.80046692	-0.0107	-108.80046699	-108.80052274	-0.0458	-109.03411981	-0.2703	-146.6194	-0.2596
3.581	-108.80046693	-0.0107	-108.80046698	-108.80051661	-0.0419	-109.03408102	-0.2460	-146.5951	-0.2353
3.631	-108.80046665	-0.0106	-108.80046669	-108.80051095	-0.0384	-109.03404609	-0.2241	-146.5733	-0.2135
3.681	-108.80046614	-0.0102	-108.80046616	-108.80050571	-0.0351	-109.03401457	-0.2043	-146.5539	-0.1941
3.731	-108.80046543	-0.0098	-108.80046545	-108.80050084	-0.0320	-109.03398610	-0.1864	-146.5365	-0.1767
3.781	-108.80046458	-0.0093	-108.80046459	-108.80049633	-0.0292	-109.03396036	-0.1703	-146.5208	-0.1610
3.831	-108.80046363	-0.0087	-108.80046364	-108.80049215	-0.0266	-109.03393707	-0.1557	-146.5068	-0.1470
3.881	-108.80046263	-0.0080	-108.80046263	-108.80048830	-0.0241	-109.03391599	-0.1425	-146.4942	-0.1344
3.931	-108.80046161	-0.0074	-108.80046161	-108.80048476	-0.0219	-109.03389689	-0.1305	-146.4829	-0.1231
3.981	-108.80046060	-0.0068	-108.80046061	-108.80048152	-0.0199	-109.03387960	-0.1196	-146.4727	-0.1129
4.031	-108.80045964	-0.0062	-108.80045964	-108.80047858	-0.0180	-109.03386394	-0.1098	-146.4634	-0.1036
4.081	-108.80045874	-0.0056	-108.80045874	-108.80047592	-0.0164	-109.03384976	-0.1009	-146.4551	-0.0953
4.131	-108.80045791	-0.0051	-108.80045791	-108.80047353	-0.0149	-109.03383692	-0.0928	-146.4476	-0.0878
4.181	-108.80045718	-0.0046	-108.80045718	-108.80047140	-0.0135	-109.03382530	-0.0855	-146.4407	-0.0809
4.231	-108.80045653	-0.0042	-108.80045653	-108.80046951	-0.0123	-109.03381477	-0.0789	-146.4345	-0.0747
4.281	-108.80045598	-0.0039	-108.80045598	-108.80046784	-0.0113	-109.03380524	-0.0730	-146.4289	-0.0691
4.331	-108.80045551	-0.0036	-108.80045551	-108.80046638	-0.0104	-109.03379660	-0.0675	-146.4238	-0.0640
4.381	-108.80045513	-0.0033	-108.80045513	-108.80046511	-0.0096	-109.03378876	-0.0626	-146.4191	-0.0593
4.431	-108.80045482	-0.0031	-108.80045482	-108.80046399	-0.0089	-109.03378164	-0.0581	-146.4148	-0.0550
4.481	-108.80045457	-0.0030	-108.80045457	-108.80046302	-0.0083	-109.03377517	-0.0541	-146.4109	-0.0511
4.531	-108.80045438	-0.0029	-108.80045438	-108.80046217	-0.0077	-109.03376929	-0.0504	-146.4073	-0.0475
4.581	-108.80045423	-0.0028	-108.80045423	-108.80046143	-0.0073	-109.03376391	-0.0470	-146.4041	-0.0443
4.681	-108.80045401	-0.0026	-108.80045401	-108.80046020	-0.0065	-109.03375448	-0.0411	-146.3983	-0.0385
4.781	-108.80045386	-0.0025	-108.80045386	-108.80045920	-0.0059	-109.03374651	-0.0361	-146.3934	-0.0336
4.881	-108.80045372	-0.0024	-108.80045372	-108.80045836	-0.0054	-109.03373970	-0.0318	-146.3892	-0.0294
4.981	-108.80045356	-0.0023	-108.80045356	-108.80045761	-0.0049	-109.03373384	-0.0282	-146.3856	-0.0258
5.081	-108.80045337	-0.0022	-108.80045337	-108.80045692	-0.0044	-109.03372875	-0.0250	-146.3825	-0.0227
5.181	-108.80045315	-0.0021	-108.80045315	-108.80045627	-0.0040	-109.03372429	-0.0222	-146.3799	-0.0201
5.281	-108.80045289	-0.0019	-108.80045289	-108.80045565	-0.0037	-109.03372037	-0.0197	-146.3776	-0.0178
5.381	-108.80045261	-0.0017	-108.80045261	-108.80045507	-0.0033	-109.03371691	-0.0175	-146.3756	-0.0158
5.481	-108.80045233	-0.0016	-108.80045233	-108.80045451	-0.0029	-109.03371385	-0.0156	-146.3738	-0.0140
5.581	-108.80045204	-0.0014	-108.80045204	-108.80045400	-0.0026	-109.03371114	-0.0139	-146.3723	-0.0125
5.681	-108.80045177	-0.0012	-108.80045177	-108.80045352	-0.0023	-109.03370874	-0.0124	-146.3710	-0.0112
5.781	-108.80045151	-0.0011	-108.80045151	-108.80045308	-0.0020	-109.03370661	-0.0111	-146.3698	-0.0100
5.881	-108.80045127	-0.0009	-108.80045127	-108.80045268	-0.0018	-109.03370472	-0.0099	-146.3688	-0.0090
5.981	-108.80045105	-0.0008	-108.80045105	-108.80045233	-0.0016	-109.03370304	-0.0088	-146.3679	-0.0081
6.081	-108.80045086	-0.0006	-108.80045086	-108.80045201	-0.0014	-109.03370156	-0.0079	-146.3671	-0.0072

6.181		-108.80045069	-0.0005	-108.80045069	-108.80045173	-0.0012	-109.03370024	-0.0071	-146.3663	-0.0065
6.281		-108.80045054	-0.0004	-108.80045054	-108.80045149	-0.0010	-109.03369907	-0.0063	-146.3657	-0.0059
6.381		-108.80045041	-0.0004	-108.80045041	-108.80045127	-0.0009	-109.03369804	-0.0057	-146.3651	-0.0053
6.481		-108.80045030	-0.0003	-108.80045030	-108.80045109	-0.0008	-109.03369712	-0.0051	-146.3646	-0.0048
6.581		-108.80045021	-0.0002	-108.80045021	-108.80045093	-0.0007	-109.03369630	-0.0046	-146.3642	-0.0044
6.681		-108.80045014	-0.0002	-108.80045014	-108.80045079	-0.0006	-109.03369557	-0.0041	-146.3637	-0.0039
6.781		-108.80045008	-0.0002	-108.80045007	-108.80045067	-0.0005	-109.03369492	-0.0037	-146.3634	-0.0036
6.881		-108.80045002	-0.0001	-108.80045002	-108.80045057	-0.0005	-109.03369435	-0.0034	-146.3631	-0.0033
6.981		-108.80044998	-0.0001	-108.80044998	-108.80045048	-0.0004	-109.03369383	-0.0030	-146.3628	-0.0029
7.081		-108.80044995	-0.0001	-108.80044995	-108.80045041	-0.0004	-109.03369337	-0.0028	-146.3625	-0.0027
7.181		-108.80044992	-0.0001	-108.80044992	-108.80045034	-0.0003	-109.03369296	-0.0025	-146.3622	-0.0024
7.281		-108.80044990	0.0000	-108.80044990	-108.80045029	-0.0003	-109.03369260	-0.0023	-146.3620	-0.0022
7.381		-108.80044988	0.0000	-108.80044988	-108.80045024	-0.0003	-109.03369227	-0.0021	-146.3618	-0.0020
7.481		-108.80044987	0.0000	-108.80044987	-108.80045020	-0.0002	-109.03369197	-0.0019	-146.3617	-0.0019
7.581		-108.80044986	0.0000	-108.80044986	-108.80045016	-0.0002	-109.03369171	-0.0017	-146.3615	-0.0017
7.681		-108.80044985	0.0000	-108.80044985	-108.80045013	-0.0002	-109.03369147	-0.0016	-146.3614	-0.0015
7.781		-108.80044984	0.0000	-108.80044984	-108.80045011	-0.0002	-109.03369126	-0.0014	-146.3612	-0.0014
7.881		-108.80044984	0.0000	-108.80044984	-108.80045008	-0.0002	-109.03369107	-0.0013	-146.3611	-0.0013
7.981		-108.80044984	0.0000	-108.80044984	-108.80045006	-0.0001	-109.03369089	-0.0012	-146.3610	-0.0012
8.081		-108.80044983	0.0000	-108.80044983	-108.80045004	-0.0001	-109.03369074	-0.0011	-146.3609	-0.0011
8.181		-108.80044983	0.0000	-108.80044983	-108.80045003	-0.0001	-109.03369060	-0.0010	-146.3608	-0.0010
8.281		-108.80044983	0.0000	-108.80044983	-108.80045001	-0.0001	-109.03369047	-0.0009	-146.3607	-0.0009
8.381		-108.80044983	0.0000	-108.80044983	-108.80045000	-0.0001	-109.03369035	-0.0009	-146.3607	-0.0009
8.481		-108.80044983	0.0000	-108.80044983	-108.80044999	-0.0001	-109.03369024	-0.0008	-146.3606	-0.0008
8.581		-108.80044983	0.0000	-108.80044983	-108.80044998	-0.0001	-109.03369015	-0.0007	-146.3605	-0.0007
8.681		-108.80044983	0.0000	-108.80044983	-108.80044997	-0.0001	-109.03369006	-0.0007	-146.3605	-0.0007
8.781		-108.80044983	0.0000	-108.80044983	-108.80044996	-0.0001	-109.03368998	-0.0006	-146.3604	-0.0006
8.881		-108.80044983	0.0000	-108.80044983	-108.80044995	-0.0001	-109.03368991	-0.0006	-146.3604	-0.0006
8.981		-108.80044983	0.0000	-108.80044983	-108.80044994	-0.0001	-109.03368984	-0.0005	-146.3603	-0.0005
9.081		-108.80044983	0.0000	-108.80044983	-108.80044993	-0.0001	-109.03368978	-0.0005	-146.3603	-0.0005
9.181		-108.80044983	0.0000	-108.80044983	-108.80044993	-0.0001	-109.03368975	-0.0005	-146.3603	-0.0005
9.281		-108.80044983	0.0000	-108.80044983	-108.80044992	-0.0001	-109.03368969	-0.0004	-146.3603	-0.0004
9.381		-108.80044983	0.0000	-108.80044983	-108.80044991	-0.0001	-109.03368965	-0.0004	-146.3602	-0.0004
9.481		-108.80044983	0.0000	-108.80044983	-108.80044991	-0.0001	-109.03368960	-0.0004	-146.3602	-0.0004
9.581		-108.80044983	0.0000	-108.80044983	-108.80044990	0.0000	-109.03368956	-0.0004	-146.3602	-0.0004
20.000		-108.80044983	0.0000	-108.80044983	-108.80044983	0.0000	-109.03368898	0.0000	-146.3598	0.0000

Re		
1.101		
DCF (Re-shifted)		
ΔR	vCASC13-SCGVB	$\Delta(vCASC13-SCGVB)$
-0.330	-193.7846	-47.4248
-0.320	-193.9342	-47.5744
-0.310	-194.0902	-47.7304
-0.300	-194.2521	-47.8922
-0.290	-194.4196	-48.0598
-0.280	-194.5924	-48.2326
-0.270	-194.7702	-48.4104
-0.260	-194.9527	-48.5929
-0.250	-195.1395	-48.7797
-0.240	-195.3303	-48.9704
-0.230	-195.5247	-49.1649
-0.220	-195.7225	-49.3627
-0.210	-195.9232	-49.5634
-0.200	-196.1266	-49.7668
-0.190	-196.3322	-49.9724
-0.180	-196.5397	-50.1799
-0.160	-196.9588	-50.5990
-0.140	-197.3807	-51.0209
-0.120	-197.8021	-51.4423
-0.100	-198.2196	-51.8598
-0.080	-198.6294	-52.2696
-0.060	-199.0279	-52.6681
-0.040	-199.4111	-53.0512
-0.020	-199.7746	-53.4148
0.000	-200.1142	-53.7544
0.020	-200.4254	-54.0656
0.040	-200.7033	-54.3435
0.060	-200.9433	-54.5835
0.080	-201.1402	-54.7804
0.100	-201.2890	-54.9292
0.120	-201.3846	-55.0248
0.140	-201.4220	-55.0622
0.160	-201.3961	-55.0363
0.180	-201.3019	-54.9421
0.200	-201.1349	-54.7751
0.220	-200.8906	-54.5308
0.240	-200.5650	-54.2052
0.260	-200.1545	-53.7947
0.280	-199.6561	-53.2963
0.300	-199.0675	-52.7077
0.320	-198.3871	-52.0273
0.340	-197.6142	-51.2544
0.360	-196.7490	-50.3892
0.380	-195.7928	-49.4330
0.400	-194.7477	-48.3879
0.420	-193.6173	-47.2575
0.440	-192.4060	-46.0462
0.460	-191.1193	-44.7595
0.480	-189.7639	-43.4041
0.500	-188.3472	-41.9874
0.520	-186.8775	-40.5177
0.540	-185.3639	-39.0041
0.560	-183.8159	-37.4561
0.580	-182.2433	-35.8835
0.600	-180.6562	-34.2964
0.620	-179.0644	-32.7046
0.640	-177.4776	-31.1178
0.660	-175.9051	-29.5453
0.680	-174.3556	-27.9958
0.700	-172.8371	-26.4773
0.720	-171.3568	-24.9970
0.740	-169.9208	-23.5610
0.760	-168.5345	-22.1747
0.780	-167.2022	-20.8424
0.800	-165.9271	-19.5673

0.820	-164.7115	-18.3517
0.840	-163.5569	-17.1971
0.860	-162.4638	-16.1040
0.880	-161.4321	-15.0723
0.900	-160.4608	-14.1010
0.920	-159.5486	-13.1888
0.940	-158.6936	-12.3338
0.960	-157.8936	-11.5338
0.980	-157.1462	-10.7864
1.030	-155.4905	-9.1307
1.080	-154.1046	-7.7448
1.130	-152.9473	-6.5875
1.180	-151.9810	-5.6212
1.230	-151.1731	-4.8133
1.280	-150.4959	-4.1361
1.330	-149.9265	-3.5667
1.380	-149.4461	-3.0863
1.430	-149.0392	-2.6794
1.480	-148.6933	-2.3335
1.530	-148.3982	-2.0384
1.580	-148.1454	-1.7856
1.630	-147.9282	-1.5684
1.680	-147.7409	-1.3811
1.730	-147.5789	-1.2191
1.780	-147.4384	-1.0786
1.830	-147.3161	-0.9563
1.880	-147.2095	-0.8497
1.930	-147.1162	-0.7564
1.980	-147.0345	-0.6747
2.030	-146.9626	-0.6028
2.080	-146.8994	-0.5396
2.130	-146.8435	-0.4837
2.180	-146.7942	-0.4344
2.230	-146.7505	-0.3907
2.280	-146.7118	-0.3520
2.330	-146.6774	-0.3175
2.380	-146.6467	-0.2869
2.430	-146.6194	-0.2596
2.480	-146.5951	-0.2353
2.530	-146.5733	-0.2135
2.580	-146.5539	-0.1941
2.630	-146.5365	-0.1767
2.680	-146.5208	-0.1610
2.730	-146.5068	-0.1470
2.780	-146.4942	-0.1344
2.830	-146.4829	-0.1231
2.880	-146.4727	-0.1129
2.930	-146.4634	-0.1036
2.980	-146.4551	-0.0953
3.030	-146.4476	-0.0878
3.080	-146.4407	-0.0809
3.130	-146.4345	-0.0747
3.180	-146.4289	-0.0691
3.230	-146.4238	-0.0640
3.280	-146.4191	-0.0593
3.330	-146.4148	-0.0550
3.380	-146.4109	-0.0511
3.430	-146.4073	-0.0475
3.480	-146.4041	-0.0443
3.580	-146.3983	-0.0385
3.680	-146.3934	-0.0336
3.780	-146.3892	-0.0294
3.880	-146.3856	-0.0258
3.980	-146.3825	-0.0227
4.080	-146.3799	-0.0201
4.180	-146.3776	-0.0178
4.280	-146.3756	-0.0158
4.380	-146.3738	-0.0140
4.480	-146.3723	-0.0125
4.580	-146.3710	-0.0112
4.680	-146.3698	-0.0100
4.780	-146.3688	-0.0090
4.880	-146.3679	-0.0081
4.980	-146.3671	-0.0072

5.080	-146.3663	-0.0065
5.180	-146.3657	-0.0059
5.280	-146.3651	-0.0053
5.380	-146.3646	-0.0048
5.480	-146.3642	-0.0044
5.580	-146.3637	-0.0039
5.680	-146.3634	-0.0036
5.780	-146.3631	-0.0033
5.880	-146.3628	-0.0029
5.980	-146.3625	-0.0027
6.080	-146.3622	-0.0024
6.180	-146.3620	-0.0022
6.280	-146.3618	-0.0020
6.380	-146.3617	-0.0019
6.480	-146.3615	-0.0017
6.580	-146.3614	-0.0015
6.680	-146.3612	-0.0014
6.780	-146.3611	-0.0013
6.880	-146.3610	-0.0012
6.980	-146.3609	-0.0011
7.080	-146.3608	-0.0010
7.180	-146.3607	-0.0009
7.280	-146.3607	-0.0009
7.380	-146.3606	-0.0008
7.480	-146.3605	-0.0007
7.580	-146.3605	-0.0007
7.680	-146.3604	-0.0006
7.780	-146.3604	-0.0006
7.880	-146.3603	-0.0005
7.980	-146.3603	-0.0005
8.080	-146.3603	-0.0005
8.180	-146.3603	-0.0004
8.280	-146.3602	-0.0004
8.380	-146.3602	-0.0004
8.480	-146.3602	-0.0004
18.899	-146.3598	0.0000

O2: RHF, CCSD(T), SCGVb, vCAS and vCASCI ENERGIES

R(Å)	E(R=∞)		E(R=∞)		E(R=20.0)		E(R=20.0)		E(R=20.0)		DCE(R=20.0)			
	-149.622129		-149.989862		-149.62064662		-149.61795785		-149.61795785		-149.96151730		-213.8996	
	E(RHF)	ΔE(RHF)	E[CCSD(T)]	ΔE[CCSD(T)]	SCGVb(2)	ΔE(SCGVb(2))	vCAS3: (occ,3,1,1,0,3,1,1,0;closed,2,0,0,0,2,0,0,0) + (occ,3,1,1,0,3,1,1,0;closed,1,0,0,0,1,0,0,0,0;frozen DCE	E(vCAS1)	E(vCAS3)	ΔE(vCAS3)	E(vCASCI3)	ΔE(vCASCI3)	vCASCI3-SCGVb(2)	Δ(vCASCI3-SCGVb(2))
0.878					-149.37175037	156.1848	-149.38903752	-149.39206207	141.7518	-149.77813742	115.0726	-255.0118	-41.1122	
0.888					-149.40392739	135.9934	-149.42173495	-149.42483663	121.1854	-149.81059877	94.7028	-255.1902	-41.2906	
0.898					-149.43378197	117.2594	-149.45211516	-149.45529389	102.0732	-149.84074703	75.7845	-255.3745	-41.4749	
0.908					-149.46145580	99.8938	-149.48031959	-149.48357530	84.3263	-149.86872364	58.2289	-255.5645	-41.6649	
0.918					-149.48708211	83.8130	-149.50648124	-149.50981379	67.8614	-149.89466152	41.9526	-255.7600	-41.8604	
0.928					-149.51078623	68.9384	-149.53072510	-149.53413434	52.6001	-149.91868560	26.8773	-255.9608	-42.0611	
0.938					-149.53268604	55.1961	-149.55316874	-149.55665444	38.4685	-149.94091334	12.9292	-256.1665	-42.2669	
0.948					-149.55289249	42.5164	-149.57392268	-149.57748459	25.3974	-149.96145518	0.0390	-256.3770	-42.4774	
0.958					-149.57150996	30.8337	-149.59309088	-149.59672871	13.3215	-149.98041498	-11.8585	-256.5918	-42.6922	
0.968					-149.58863673	20.0865	-149.61077113	-149.61448452	2.1795	-149.99789043	-22.8245	-256.8106	-42.9110	
0.978					-149.60436532	10.2167	-149.62705544	-149.63084398	-0.8062	-150.01397342	-32.9167	-257.0330	-43.1334	
0.988					-149.61878285	1.1695	-149.64203033	-149.64589357	-17.5299	-150.02875038	-42.1894	-257.2586	-43.3589	
0.998					-149.63197137	-7.1064	-149.65577725	-149.65971466	-26.2028	-150.04230265	-50.6936	-257.4868	-43.5872	
1.008					-149.64400818	-14.6596	-149.66837282	-149.67238382	-34.1528	-150.05470673	-58.4773	-257.7173	-43.8177	
1.018					-149.65496608	-21.5358	-149.67988914	-149.68397309	-41.4252	-150.06630463	-65.5856	-257.9495	-44.0498	
1.028					-149.66491370	-27.7780	-149.69039406	-149.69455026	-48.0625	-150.07635410	-72.0612	-258.1828	-44.2832	
1.048					-149.68203300	-38.5205	-149.70862134	-149.71291967	-59.5895	-150.09421894	-83.2716	-258.6506	-44.7510	
1.068					-149.69584000	-47.1846	-149.72352161	-149.72795848	-69.0265	-150.10876735	-92.4008	-259.1159	-45.2163	
1.088					-149.70675586	-54.0344	-149.73550831	-149.74007960	-76.6326	-150.12041194	-99.7079	-259.5732	-45.6735	
1.108					-149.71515486	-59.3048	-149.74494746	-149.74964850	-82.6371	-150.12951782	-105.4219	-260.0167	-46.1171	
1.128	-149.66977248	-29.8968	-150.16724180	-111.3076	-149.72136971	-63.2047	-149.75216293	-149.75698854	-87.2431	-150.13640793	-109.7455	-260.4405	-46.5408	
1.148	-149.67095500	-30.6388	-150.17225230	-114.4517	-149.72569610	-65.9196	-149.75744120	-149.76238563	-90.6298	-150.14136775	-112.8579	-260.8380	-46.9383	
1.168	-149.67035667	-30.2634	-150.17556971	-116.5334	-149.72839673	-67.6142	-149.76103553	-149.76609250	-92.9559	-150.14464943	-114.9172	-261.2026	-47.3029	
1.188	-149.66820491	-28.9131	-150.17741541	-117.6916	-149.72970484	-68.4351	-149.76316965	-149.76833237	-94.3615	-150.14647551	-116.0631	-261.5276	-47.6280	
1.208	-149.66470122	-26.7145	-150.17798454	-118.0487	-149.72982736	-68.5120	-149.76404115	-149.76930230	-94.9701	-150.14704225	-116.4187	-261.8063	-47.9067	
1.228	-149.66002409	-23.7796	-150.17744893	-117.7126	-149.72894765	-67.9599	-149.76382439	-149.76917612	-94.8909	-150.14652257	-116.0926	-262.0323	-48.1326	
1.248	-149.65433160	-20.2075	-150.17595976	-116.7782	-149.72722791	-66.8808	-149.76267320	-149.76810719	-94.2202	-150.14506874	-115.1803	-262.1991	-48.2995	
1.268	-149.64776371	-16.0861	-150.17364993	-115.3287	-149.72481143	-65.3644	-149.76072322	-149.76623066	-93.0426	-150.14281473	-113.7659	-262.3011	-48.4015	
1.288	-149.64044429	-11.4931	-150.17063563	-113.4372	-149.72182447	-63.4901	-149.75809409	-149.76366573	-91.4331	-150.13987837	-111.9233	-262.3328	-48.4332	
1.308					-149.71837802	-61.3274	-149.75489131	-149.76051747	-89.4575	-150.13636326	-109.7175	-262.2898	-48.3901	
1.328					-149.71456943	-58.9375	-149.75120796	-149.75687857	-87.1741	-150.13236049	-107.2057	-262.1679	-48.2683	
1.348					-149.71048377	-56.3737	-149.74712618	-149.75283082	-84.6341	-150.12795018	-104.4382	-261.9642	-48.0646	
1.368					-149.70619514	-53.6825	-149.74271855	-149.74844649	-81.8829	-150.12320280	-101.4592	-261.6763	-47.7767	
1.388					-149.70176789	-50.9044	-149.73804924	-149.74378950	-78.9606	-150.11818043	-98.3076	-261.3029	-47.4032	
1.408					-149.69725760	-48.0741	-149.73317507	-149.73891645	-75.9027	-150.11293778	-95.0178	-260.8433	-46.9437	
1.428					-149.69271211	-45.2218	-149.72814637	-149.73387752	-72.7407	-150.10752313	-91.6201	-260.2979	-46.3983	
1.448					-149.68817235	-42.3730	-149.72300785	-149.72871733	-69.5026	-150.10197918	-88.1412	-259.6678	-45.7681	
1.468					-149.68367312	-39.5497	-149.71779923	-149.72347554	-66.2134	-150.09634371	-84.6049	-258.9548	-45.0551	
1.488					-149.67924382	-36.7703	-149.71255588	-149.71818753	-62.8951	-150.09065026	-81.0322	-258.1615	-44.2619	
1.508					-149.67490909	-34.0502	-149.70730933	-149.71288490	-59.5676	-150.08492864	-77.4418	-257.2912	-43.3916	
1.528					-149.67068938	-31.4023	-149.70208772	-149.70759590	-56.2487	-150.07920539	-73.8504	-256.3477	-42.4481	
1.548					-149.66660148	-28.8371	-149.69691620	-149.70234584	-52.9543	-150.07350422	-70.2729	-255.3354	-41.4358	
1.568					-149.66265900	-26.3632	-149.69181727	-149.69715746	-49.6985	-150.06784633	-66.7225	-254.2589	-40.3593	
1.588					-149.65887276	-23.9873	-149.68681109	-149.69205117	-46.4943	-150.06225073	-63.2112	-253.1235	-39.2239	
1.608					-149.65525121	-21.7147	-149.68191572	-149.68704535	-43.3531	-150.05673456	-59.7497	-251.9347	-38.0350	
1.628					-149.65180072	-19.5495	-149.67714737	-149.68215655	-40.2853	-150.05131317	-56.3478	-250.6979	-36.7983	
1.648					-149.64852590	-17.4945	-149.67252054	-149.67739969	-37.3003	-150.04600051	-53.0140	-249.4191	-35.5195	
1.668					-149.64542982	-15.5517	-149.66804824	-149.67278823	-34.4066	-150.04080918	-49.7564	-248.1043	-34.2047	
1.688					-149.64251424	-13.7221	-149.66374207	-149.66833430	-31.6117	-150.03575061	-46.5821	-246.7596	-32.8600	
1.708					-149.63977976	-12.0062	-149.65961238	-149.66404878	-28.9225	-150.03083522	-43.4977	-245.3911	-31.4914	
1.728					-149.63722593	-10.4037	-149.65566829	-149.65994145	-26.3451	-150.02607248	-40.5090	-244.0049	-30.1053	
1.748					-149.63485142	-8.9136	-149.65191776	-149.65602097	-23.8850	-150.02147102	-37.6215	-242.6075	-28.7079	
1.768					-149.63265399	-7.5347	-149.64836762	-149.65229494	-21.5469	-150.01703868	-34.8402	-241.2051	-27.3055	
1.788					-149.63063063	-6.2651	-149.64502353	-149.64876991	-19.3349	-150.01278262	-32.1695	-239.8040	-25.9044	
1.808					-149.62877751	-5.1022	-149.64188994	-149.64545128	-17.2524	-150.00870924	-29.6134	-238.4108	-24.5112	
1.828					-149.62709004	-4.0433	-149.63897003	-149.64234331	-15.3021	-150.00482437	-27.1756	-237.0319	-23.1323	
1.848					-149.62556286	-3.0850	-149.63626557	-149.63944893	-13.4859	-150.00113306	-24.8593	-235.6739	-21.7743	
1.868					-149.62418988	-2.2234	-149.63377683	-149.63676968	-11.8046	-149.99763964	-22.6671	-234.3433	-20.4437	
1.888					-149.62296425	-1.4543	-149.63150241	-149.63430553	-10.2583	-149.99434764	-20.6014	-233.0466	-19.1470	
1.908					-149.62187848	-0.7730	-149.62943917	-149.63205474	-8.8459	-149.99125968	-18.6636	-231.7902	-17.8906	
1.928					-149.62092443	-0.1743	-149.62758213	-149.63001376	-7.5652	-149.98837730	-16.8549	-230.5802	-16.6806	
1.948					-149.62009370	0.3470	-149.62592442	-149.62817714	-6.4127	-149.98570083	-15.1754	-229.4220	-15.5224	
1.968					-149.61988585	0.4774	-149.62445736	-149.62653755	-5.3838	-149.98322915	-13.6244	-228.0014	-14.1018	
1.988					-149.61909646	0.9727	-149.62317064	-149.62508585	-4.4729	-149.98095959	-12.2002	-227.0726	-13.1730	
2.008					-149.61883493	1.1369	-149.62205247	-149.62381126	-3.6731	-149.97888773	-10.9001	-225.9366	-12.0370	

2.028	-149.61863568	1.2619	-149.62109000	-149.62270170	-2.9768	-149.97700740	-9.7202	-224.8817	-10.9821
2.048	-149.61848949	1.3536	-149.62026963	-149.62174409	-2.3759	-149.97531069	-8.6555	-223.9087	-10.0091
2.068	-149.61838917	1.4166	-149.61957745	-149.62092473	-1.8617	-149.97378810	-7.7000	-223.0162	-9.1166
2.088	-149.61832809	1.4549	-149.61899959	-149.62022977	-1.4257	-149.97242882	-6.8471	-222.2016	-8.3020
2.108	-149.61830020	1.4724	-149.61852257	-149.61964550	-1.0590	-149.97122105	-6.0892	-221.4612	-7.5616
2.128	-149.61830006	1.4725	-149.61813359	-149.61915875	-0.7536	-149.97015241	-5.4186	-220.7907	-6.8911
2.148	-149.61832278	1.4582	-149.61782075	-149.61875706	-0.5015	-149.96921025	-4.8274	-220.1853	-6.2856
2.168	-149.61836406	1.4323	-149.61757312	-149.61842893	-0.2956	-149.96838209	-4.3077	-219.6397	-5.7400
2.188	-149.61842010	1.3972	-149.61738089	-149.61816386	-0.1293	-149.96765583	-3.8520	-219.1488	-5.2491
2.238	-149.61860437	1.2815	-149.61708780	-149.61771798	0.1505	-149.96621285	-2.9465	-218.1277	-4.2280
2.288	-149.61882193	1.1450	-149.61697996	-149.61749148	0.2927	-149.96518182	-2.2995	-217.3442	-3.4445
2.338	-149.61904693	1.0038	-149.61698218	-149.61740100	0.3494	-149.96444220	-1.8354	-216.7388	-2.8392
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2.438	-149.61946320	0.7426	-149.61713688	-149.61742429	0.3348	-149.96350978	-1.2503	-215.8925	-1.9929
2.488	-149.61964165	0.6306	-149.61723884	-149.61747929	0.3003	-149.96321124	-1.0630	-215.5932	-1.6936
2.538	-149.61979787	0.5326	-149.61733975	-149.61754200	0.2609	-149.96298052	-0.9182	-215.3504	-1.4508
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2.638	-149.62004744	0.3760	-149.61751789	-149.61766287	0.1851	-149.96264895	-0.7101	-214.9857	-1.0861
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2.888	-149.62040021	0.1546	-149.61779194	-149.61785858	0.0623	-149.96218278	-0.4176	-214.4718	-0.5722
2.938	-149.62044013	0.1296	-149.61782349	-149.61788097	0.0482	-149.96212136	-0.3791	-214.4083	-0.5086
2.988	-149.62047339	0.1087	-149.61784962	-149.61789929	0.0367	-149.96206652	-0.3446	-214.3530	-0.4533
3.038	-149.62050105	0.0913	-149.61787114	-149.61791416	0.0274	-149.96201732	-0.3138	-214.3047	-0.4051
3.088	-149.62052402	0.0769	-149.61788876	-149.61792611	0.0199	-149.96197300	-0.2860	-214.2625	-0.3629
3.138	-149.62054305	0.0650	-149.61790310	-149.61793559	0.0140	-149.96193294	-0.2608	-214.2254	-0.3258
3.188	-149.62055878	0.0551	-149.61791467	-149.61794300	0.0093	-149.96189665	-0.2380	-214.1928	-0.2932
3.238	-149.62057173	0.0470	-149.61792394	-149.61794870	0.0057	-149.96186370	-0.2174	-214.1640	-0.2644
3.288	-149.62058237	0.0403	-149.61793129	-149.61795297	0.0031	-149.96183374	-0.1986	-214.1385	-0.2389
3.338	-149.62059108	0.0349	-149.61793705	-149.61795609	0.0011	-149.96180648	-0.1815	-214.1159	-0.2163
3.388	-149.62059820	0.0304	-149.61794151	-149.61795827	-0.0003	-149.96178165	-0.1659	-214.0959	-0.1963
3.438	-149.62060401	0.0267	-149.61794492	-149.61795971	-0.0012	-149.96175904	-0.1517	-214.0781	-0.1784
3.488	-149.62060876	0.0238	-149.61794750	-149.61796058	-0.0017	-149.96173846	-0.1388	-214.0622	-0.1625
3.538	-149.62061267	0.0213	-149.61794942	-149.61796103	-0.0020	-149.96171975	-0.1270	-214.0480	-0.1483
3.588	-149.62061590	0.0193	-149.61795086	-149.61796118	-0.0021	-149.96170275	-0.1164	-214.0353	-0.1356
3.638	-149.62061860	0.0176	-149.61795192	-149.61796113	-0.0021	-149.96168732	-0.1067	-214.0239	-0.1243
3.688	-149.62062091	0.0161	-149.61795273	-149.61796096	-0.0020	-149.96167334	-0.0979	-214.0137	-0.1140
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3.838	-149.62062628	0.0128	-149.61795431	-149.61796028	-0.0015	-149.96163890	-0.0763	-213.9887	-0.0891
3.888	-149.62062775	0.0118	-149.61795471	-149.61796010	-0.0014	-149.96162956	-0.0704	-213.9819	-0.0823
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4.088	-149.62063279	0.0087	-149.61795623	-149.61795991	-0.0013	-149.96160031	-0.0521	-213.9604	-0.0608
4.138	-149.62063389	0.0080	-149.61795660	-149.61795996	-0.0013	-149.96159461	-0.0485	-213.9561	-0.0565
4.188	-149.62063491	0.0073	-149.61795695	-149.61796003	-0.0014	-149.96158941	-0.0452	-213.9522	-0.0526
4.238	-149.62063588	0.0067	-149.61795728	-149.61796011	-0.0014	-149.96158465	-0.0423	-213.9486	-0.0490
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4.438	-149.62063904	0.0048	-149.61795832	-149.61796037	-0.0016	-149.96156909	-0.0325	-213.9369	-0.0373
4.488	-149.62063965	0.0044	-149.61795849	-149.61796039	-0.0016	-149.96156589	-0.0305	-213.9345	-0.0349
4.538	-149.62064020	0.0040	-149.61795863	-149.61796038	-0.0016	-149.96156290	-0.0286	-213.9323	-0.0326
4.588	-149.62064069	0.0037	-149.61795873	-149.61796036	-0.0016	-149.96156011	-0.0269	-213.9302	-0.0306
4.638	-149.62064113	0.0034	-149.61795879	-149.61796031	-0.0015	-149.96155750	-0.0252	-213.9283	-0.0287
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4.738	-149.62064213	0.0028	-149.61795883	-149.61796006	-0.0014	-149.96155060	-0.0209	-213.9233	-0.0237
4.788	-149.62064260	0.0025	-149.61795876	-149.61795983	-0.0012	-149.96154668	-0.0184	-213.9206	-0.0210
4.838	-149.62064295	0.0023	-149.61795863	-149.61795958	-0.0011	-149.96154322	-0.0163	-213.9182	-0.0186
4.888	-149.62064322	0.0021	-149.61795848	-149.61795931	-0.0009	-149.96154016	-0.0143	-213.9161	-0.0165
4.938	-149.62064344	0.0020	-149.61795831	-149.61795905	-0.0008	-149.96153746	-0.0127	-213.9143	-0.0146
4.988	-149.62064361	0.0019	-149.61795815	-149.61795881	-0.0006	-149.96153509	-0.0112	-213.9127	-0.0131
5.038	-149.62064375	0.0018	-149.61795800	-149.61795858	-0.0005	-149.96153299	-0.0098	-213.9113	-0.0116
5.088	-149.62064388	0.0017	-149.61795786	-149.61795838	-0.0003	-149.96153115	-0.0087	-213.9100	-0.0104
5.138	-149.62064399	0.0017	-149.61795774	-149.61795820	-0.0002	-149.96152952	-0.0077	-213.9089	-0.0093
5.188	-149.62064410	0.0016	-149.61795763	-149.61795805	-0.0001	-149.96152809	-0.0068	-213.9080	-0.0084
5.238	-149.62064420	0.0015	-149.61795754	-149.61795791	0.0000	-149.96152682	-0.0060	-213.9071	-0.0075
5.288	-149.62064429	0.0015	-149.61795746	-149.61795780	0.0000	-149.96152571	-0.0053	-213.9064	-0.0067
5.338	-149.62064439	0.0014	-149.61795740	-149.61795770	0.0001	-149.96152473	-0.0047	-213.9057	-0.0061
5.388	-149.62064448	0.0013	-149.61795735	-149.61795763	0.0001	-149.96152387	-0.0041	-213.9051	-0.0055
5.438	-149.62064457	0.0013	-149.61795732	-149.61795756	0.0002	-149.96152311	-0.0036	-213.9046	-0.0049

6.288		-149.62064466	0.0012	-149.61795729	-149.61795752	0.0002	-149.96152245	-0.0032	-213.9041	-0.0045
6.388		-149.62064475	0.0012	-149.61795727	-149.61795748	0.0002	-149.96152186	-0.0029	-213.9037	-0.0040
6.488		-149.62064484	0.0011	-149.61795727	-149.61795745	0.0003	-149.96152135	-0.0025	-213.9033	-0.0037
6.588		-149.62064493	0.0011	-149.61795727	-149.61795744	0.0003	-149.96152092	-0.0023	-213.9030	-0.0033
6.688		-149.62064501	0.0010	-149.61795727	-149.61795743	0.0003	-149.96152052	-0.0020	-213.9027	-0.0030
6.788		-149.62064510	0.0010	-149.61795729	-149.61795743	0.0003	-149.96152018	-0.0018	-213.9024	-0.0028
6.888		-149.62064518	0.0009	-149.61795730	-149.61795743	0.0003	-149.96151987	-0.0016	-213.9021	-0.0025
6.988		-149.62064526	0.0009	-149.61795732	-149.61795744	0.0003	-149.96151961	-0.0014	-213.9019	-0.0023
7.088		-149.62064534	0.0008	-149.61795734	-149.61795745	0.0003	-149.96151937	-0.0013	-213.9017	-0.0021
7.188		-149.62064541	0.0008	-149.61795736	-149.61795746	0.0002	-149.96151917	-0.0012	-213.9016	-0.0019
7.288		-149.62064549	0.0007	-149.61795739	-149.61795748	0.0002	-149.96151899	-0.0011	-213.9014	-0.0018
7.388		-149.62064555	0.0007	-149.61795741	-149.61795749	0.0002	-149.96151883	-0.0010	-213.9013	-0.0016
7.488		-149.62064562	0.0006	-149.61795743	-149.61795751	0.0002	-149.96151868	-0.0009	-213.9011	-0.0015
7.588		-149.62064568	0.0006	-149.61795746	-149.61795753	0.0002	-149.96151856	-0.0008	-213.9010	-0.0014
7.688		-149.62064573	0.0006	-149.61795748	-149.61795754	0.0002	-149.96151845	-0.0007	-213.9009	-0.0013
7.788		-149.62064579	0.0005	-149.61795750	-149.61795756	0.0002	-149.96151835	-0.0007	-213.9008	-0.0012
7.888		-149.62064584	0.0005	-149.61795752	-149.61795758	0.0002	-149.96151826	-0.0006	-213.9007	-0.0011
7.988		-149.62064589	0.0005	-149.61795754	-149.61795759	0.0002	-149.96151818	-0.0006	-213.9006	-0.0010
8.088		-149.62064593	0.0004	-149.61795756	-149.61795760	0.0002	-149.96151811	-0.0005	-213.9006	-0.0009
8.188		-149.62064597	0.0004	-149.61795757	-149.61795762	0.0001	-149.96151804	-0.0005	-213.9005	-0.0009
8.288		-149.62064601	0.0004	-149.61795759	-149.61795763	0.0001	-149.96151799	-0.0004	-213.9004	-0.0008
8.388		-149.62064604	0.0004	-149.61795760	-149.61795764	0.0001	-149.96151793	-0.0004	-213.9004	-0.0008
8.488		-149.62064608	0.0003	-149.61795762	-149.61795765	0.0001	-149.96151789	-0.0004	-213.9003	-0.0007
8.588		-149.62064611	0.0003	-149.61795763	-149.61795767	0.0001	-149.96151784	-0.0003	-213.9003	-0.0007
8.688		-149.62064614	0.0003	-149.61795764	-149.61795768	0.0001	-149.96151780	-0.0003	-213.9002	-0.0006
8.788		-149.62064617	0.0003	-149.61795766	-149.61795769	0.0001	-149.96151777	-0.0003	-213.9002	-0.0006
8.888		-149.62064619	0.0003	-149.61795767	-149.61795769	0.0001	-149.96151773	-0.0003	-213.9002	-0.0005
8.988		-149.62064622	0.0003	-149.61795768	-149.61795770	0.0001	-149.96151770	-0.0003	-213.9001	-0.0005
9.088		-149.62064624	0.0002	-149.61795769	-149.61795771	0.0001	-149.96151768	-0.0002	-213.9001	-0.0005
9.188		-149.62064626	0.0002	-149.61795770	-149.61795772	0.0001	-149.96151765	-0.0002	-213.9001	-0.0004
9.288		-149.62064628	0.0002	-149.61795770	-149.61795772	0.0001	-149.96151763	-0.0002	-213.9000	-0.0004
9.388		-149.62064630	0.0002	-149.61795771	-149.61795773	0.0001	-149.96151760	-0.0002	-213.9000	-0.0004
9.488		-149.62064631	0.0002	-149.61795772	-149.61795774	0.0001	-149.96151758	-0.0002	-213.9000	-0.0004
9.588		-149.62064633	0.0002	-149.61795773	-149.61795774	0.0001	-149.96151757	-0.0002	-213.9000	-0.0004
9.688		-149.62064635	0.0002	-149.61795773	-149.61795775	0.0001	-149.96151755	-0.0002	-213.9000	-0.0003
20.000		-149.62064662	0.0000	-149.61795785	-149.61795785	0.0000	-149.96151730	0.0000	-213.8996	0.0000

Re		
1.208		
DCE(2) (Re-shifted)		
AR	vCASC13-SCGVB(2)	Δ(vCASC13-SCGVB(2))
-0.330	-255.0118	-41.1122
-0.320	-255.1902	-41.2906
-0.310	-255.3745	-41.4749
-0.300	-255.5645	-41.6649
-0.290	-255.7600	-41.8604
-0.280	-255.9608	-42.0611
-0.270	-256.1665	-42.2669
-0.260	-256.3770	-42.4774
-0.250	-256.5918	-42.6922
-0.240	-256.8106	-42.9110
-0.230	-257.0330	-43.1334
-0.220	-257.2586	-43.3589
-0.210	-257.4868	-43.5872
-0.200	-257.7173	-43.8177
-0.190	-257.9495	-44.0498
-0.180	-258.1828	-44.2832
-0.160	-258.6506	-44.7510
-0.140	-259.1159	-45.2163
-0.120	-259.5732	-45.6735
-0.100	-260.0167	-46.1171
-0.080	-260.4405	-46.5408
-0.060	-260.8380	-46.9383
-0.040	-261.2026	-47.3029
-0.020	-261.5276	-47.6280
0.000	-261.8063	-47.9067
0.020	-262.0323	-48.1326
0.040	-262.1991	-48.2995
0.060	-262.3011	-48.4015
0.080	-262.3328	-48.4332
0.100	-262.2898	-48.3901
0.120	-262.1679	-48.2683
0.140	-261.9642	-48.0646
0.160	-261.6763	-47.7767
0.180	-261.3029	-47.4032
0.200	-260.8433	-46.9437
0.220	-260.2979	-46.3983
0.240	-259.6678	-45.7681
0.260	-258.9548	-45.0551
0.280	-258.1615	-44.2619
0.300	-257.2912	-43.3916
0.320	-256.3477	-42.4481
0.340	-255.3354	-41.4358
0.360	-254.2589	-40.3593
0.380	-253.1235	-39.2239
0.400	-251.9347	-38.0350
0.420	-250.6979	-36.7983
0.440	-249.4191	-35.5195
0.460	-248.1043	-34.2047
0.480	-246.7596	-32.8600
0.500	-245.3911	-31.4914
0.520	-244.0049	-30.1053
0.540	-242.6075	-28.7079
0.560	-241.2051	-27.3055
0.580	-239.8040	-25.9044
0.600	-238.4108	-24.5112
0.620	-237.0319	-23.1323
0.640	-235.6739	-21.7743
0.660	-234.3433	-20.4437
0.680	-233.0466	-19.1470
0.700	-231.7902	-17.8906
0.720	-230.5802	-16.6806
0.740	-229.4220	-15.5224
0.760	-228.0014	-14.1018
0.780	-227.0726	-13.1730
0.800	-225.9366	-12.0370

0.820	-224.8817	-10.9821
0.840	-223.9087	-10.0091
0.860	-223.0162	-9.1166
0.880	-222.2016	-8.3020
0.900	-221.4612	-7.5616
0.920	-220.7907	-6.8911
0.940	-220.1853	-6.2856
0.960	-219.6397	-5.7400
0.980	-219.1488	-5.2491
1.030	-218.1277	-4.2280
1.080	-217.3442	-3.4445
1.130	-216.7388	-2.8392
1.180	-216.2662	-2.3666
1.230	-215.8925	-1.9929
1.280	-215.5932	-1.6936
1.330	-215.3504	-1.4508
1.380	-215.1511	-1.2515
1.430	-214.9857	-1.0861
1.480	-214.8472	-0.9476
1.530	-214.7302	-0.8306
1.580	-214.6306	-0.7310
1.630	-214.5453	-0.6457
1.680	-214.4718	-0.5722
1.730	-214.4083	-0.5086
1.780	-214.3530	-0.4533
1.830	-214.3047	-0.4051
1.880	-214.2625	-0.3629
1.930	-214.2254	-0.3258
1.980	-214.1928	-0.2932
2.030	-214.1640	-0.2644
2.080	-214.1385	-0.2389
2.130	-214.1159	-0.2163
2.180	-214.0959	-0.1963
2.230	-214.0781	-0.1784
2.280	-214.0622	-0.1625
2.330	-214.0480	-0.1483
2.380	-214.0353	-0.1356
2.430	-214.0239	-0.1243
2.480	-214.0137	-0.1140
2.530	-214.0045	-0.1049
2.580	-213.9962	-0.0966
2.630	-213.9887	-0.0891
2.680	-213.9819	-0.0823
2.730	-213.9758	-0.0761
2.780	-213.9702	-0.0705
2.830	-213.9651	-0.0654
2.880	-213.9604	-0.0608
2.930	-213.9561	-0.0565
2.980	-213.9522	-0.0526
3.030	-213.9486	-0.0490
3.080	-213.9453	-0.0457
3.130	-213.9423	-0.0427
3.180	-213.9395	-0.0399
3.230	-213.9369	-0.0373
3.280	-213.9345	-0.0349
3.330	-213.9323	-0.0326
3.380	-213.9302	-0.0306
3.430	-213.9283	-0.0287
3.480	-213.9265	-0.0269
3.580	-213.9233	-0.0237
3.680	-213.9206	-0.0210
3.780	-213.9182	-0.0186
3.880	-213.9161	-0.0165
3.980	-213.9143	-0.0146
4.080	-213.9127	-0.0131
4.180	-213.9113	-0.0116
4.280	-213.9100	-0.0104
4.380	-213.9089	-0.0093
4.480	-213.9080	-0.0084
4.580	-213.9071	-0.0075
4.680	-213.9064	-0.0067
4.780	-213.9057	-0.0061
4.880	-213.9051	-0.0055
4.980	-213.9046	-0.0049

5.080	-213.9041	-0.0045
5.180	-213.9037	-0.0040
5.280	-213.9033	-0.0037
5.380	-213.9030	-0.0033
5.480	-213.9027	-0.0030
5.580	-213.9024	-0.0028
5.680	-213.9021	-0.0025
5.780	-213.9019	-0.0023
5.880	-213.9017	-0.0021
5.980	-213.9016	-0.0019
6.080	-213.9014	-0.0018
6.180	-213.9013	-0.0016
6.280	-213.9011	-0.0015
6.380	-213.9010	-0.0014
6.480	-213.9009	-0.0013
6.580	-213.9008	-0.0012
6.680	-213.9007	-0.0011
6.780	-213.9006	-0.0010
6.880	-213.9006	-0.0009
6.980	-213.9005	-0.0009
7.080	-213.9004	-0.0008
7.180	-213.9004	-0.0008
7.280	-213.9003	-0.0007
7.380	-213.9003	-0.0007
7.480	-213.9002	-0.0006
7.580	-213.9002	-0.0006
7.680	-213.9002	-0.0005
7.780	-213.9001	-0.0005
7.880	-213.9001	-0.0005
7.980	-213.9001	-0.0004
8.080	-213.9000	-0.0004
8.180	-213.9000	-0.0004
8.280	-213.9000	-0.0004
8.380	-213.9000	-0.0004
8.480	-213.9000	-0.0003
18.792	-213.8996	0.0000

F2: RHF, CCSD(T), SCGVB, vCAS and vCASCI ENERGIES

R(Å)	E(R=∞)		E(R=∞)		E(R=20.00)		E(R=20.0)		E(R=20.0)		E(R=20.0)		EDEC(R=20.0)	
	-198.818419		-199.305437		-198.81841799		-198.81841801		-198.81841801		-199.26920139		-282.87091102	
	E(RHF)	ΔE(RHF)	E[CCSD(T)]	ΔE[CCSD(T)]	E(SCGVB)	ΔE(SCGVB)	E(vCAS1)	E(vCAS3)	ΔE(vCAS3)	E(vCASCI3)	ΔE(vCASCI3)	vCASCI3-SCGVB	Δ(vCASCI3-SCGVB)	
1.084					-198.70182562	73.1628	-198.70394278	-198.70561823	70.7829	-199.19067640	49.2752	-306.7586	-23.8876	
1.094					-198.71335339	65.9290	-198.71549218	-198.71722458	63.4998	-199.20211765	42.0957	-306.7043	-23.8334	
1.104					-198.72411049	59.1789	-198.72626907	-198.72805691	56.7025	-199.21278251	35.4034	-306.6464	-23.7755	
1.114					-198.73414231	52.8838	-198.73631879	-198.73816037	50.3624	-199.22271554	29.1703	-306.5844	-23.7135	
1.124					-198.74349160	47.0170	-198.74568404	-198.74757747	44.4531	-199.23195868	23.3702	-306.5178	-23.6469	
1.134					-198.75219860	41.5533	-198.75440503	-198.75634826	38.9494	-199.24055147	17.9781	-306.4461	-23.5752	
1.144					-198.76030123	36.4688	-198.76251964	-198.76451046	33.8275	-199.24853113	12.9708	-306.3689	-23.4980	
1.154					-198.76783517	31.7412	-198.77006356	-198.77209963	29.0652	-199.25593276	8.3262	-306.2859	-23.4150	
1.164					-198.77483405	27.3493	-198.77707043	-198.77914929	24.6415	-199.26278946	4.0235	-306.1967	-23.3258	
1.174					-198.78132956	23.2733	-198.78357195	-198.78569104	20.5365	-199.26913245	0.0433	-306.1010	-23.2301	
1.184					-198.78735158	19.4945	-198.78959800	-198.79175468	16.7315	-199.27499118	-3.6331	-305.9985	-23.1276	
1.194					-198.79292825	15.9951	-198.79517679	-198.79736835	13.2089	-199.28039346	-7.0231	-305.8891	-23.0181	
1.204					-198.79808614	12.7584	-198.80033489	-198.80255858	9.9519	-199.28536556	-10.1432	-305.7725	-22.9016	
1.214					-198.80285028	9.7689	-198.80509740	-198.80735042	6.9450	-199.28993228	-13.0088	-305.6486	-22.7777	
1.224					-198.80724431	7.0116	-198.80948800	-198.81176752	4.1732	-199.29411707	-15.6348	-305.5173	-22.6464	
1.234					-198.81129052	4.4726	-198.81352904	-198.81583223	1.6226	-199.29794212	-18.0351	-305.3786	-22.5076	
1.254					-198.81842251	-0.0028	-198.82064569	-198.82298774	-2.8675	-199.30459571	-22.2103	-305.0784	-22.2074	
1.274					-198.82440097	-3.7544	-198.82660251	-198.82897228	-6.6229	-199.31004773	-25.6315	-304.7480	-21.8771	
1.294					-198.82936389	-6.8687	-198.83153802	-198.83392464	-9.7306	-199.31443684	-28.3857	-304.3879	-21.5170	
1.314					-198.83343447	-9.4230	-198.83557591	-198.83796897	-12.2684	-199.31788756	-30.5510	-303.9990	-21.1281	
1.334	-198.77525067	27.0883	-199.36160917	-35.2487	-198.83672273	-11.4864	-198.83882670	-198.84121634	-14.3062	-199.32051175	-32.1977	-303.5823	-20.7113	
1.354	-198.77457906	27.5098	-199.36354445	-36.4631	-198.83932694	-13.1206	-198.84138916	-198.84376613	-15.9062	-199.32241006	-33.3890	-303.1393	-20.2684	
1.374	-198.77321114	28.3682	-199.36482413	-37.2661	-198.84133488	-14.3806	-198.84335155	-198.84570729	-17.1243	-199.32367306	-34.1815	-302.6718	-19.8009	
1.394	-198.77122918	29.6119	-199.36552990	-37.7090	-198.84282493	-15.3156	-198.84479272	-198.84711940	-18.0104	-199.32438227	-34.6265	-302.1819	-19.3109	
1.414	-198.76870727	31.1944	-199.36573566	-37.8381	-198.84386705	-15.9695	-198.84578308	-198.84807362	-18.6902	-199.32461110	-34.7701	-301.6715	-18.8006	
1.434	-198.76571213	33.0739	-199.36550800	-37.6953	-198.84452363	-16.3815	-198.84638545	-198.84863352	-18.9605	-199.32442562	-34.6537	-301.1431	-18.2722	
1.454	-198.76230387	35.2126	-199.36490712	-37.3182	-198.84485026	-16.5865	-198.84665585	-198.84885586	-19.1000	-199.32388527	-34.3147	-300.5991	-17.7282	
1.474	-198.75853664	37.5766	-199.36398898	-36.7421	-198.84489642	-16.6155	-198.84664414	-198.84879123	-19.0595	-199.32304351	-33.7864	-300.0419	-17.1710	
1.494	-198.75445922	40.1352	-199.36279955	-35.9957	-198.84470604	-16.4960	-198.84639464	-198.84848468	-18.8671	-199.32194834	-33.0992	-299.4741	-16.6032	
1.514					-198.84431814	-16.2526	-198.84594671	-198.84797623	-18.5481	-199.32064280	-32.2800	-298.8983	-16.0274	
1.534					-198.84376721	-15.9069	-198.84533520	-198.84730137	-18.1246	-199.31916544	-31.3529	-298.3170	-15.4460	
1.554					-198.84308375	-15.4780	-198.84459089	-198.84649150	-17.6164	-199.31755071	-30.3397	-297.7326	-14.8617	
1.574					-198.84229457	-14.9828	-198.84374091	-198.84557428	-17.0408	-199.31582928	-29.2594	-297.1476	-14.2767	
1.594					-198.84142323	-14.4360	-198.84280907	-198.84457405	-16.4132	-199.31402839	-28.1294	-296.5643	-13.6934	
1.614					-198.84049031	-13.8506	-198.84181619	-198.84351212	-15.7468	-199.31217216	-26.9646	-295.9849	-13.1140	
1.634					-198.83951370	-13.2378	-198.84078041	-198.84240703	-15.0533	-199.31028179	-25.7783	-295.4115	-12.5406	
1.654					-198.83850889	-12.6072	-198.83971740	-198.84127486	-14.3429	-199.30837585	-24.5823	-294.8460	-11.9751	
1.674					-198.83748921	-11.9674	-198.83864066	-198.84012945	-13.6241	-199.30647050	-23.3867	-294.2903	-11.4194	
1.694					-198.83646601	-11.3253	-198.83756172	-198.83898263	-12.9045	-199.30457966	-22.2002	-293.7458	-10.8749	
1.714					-198.83544889	-10.6871	-198.83649030	-198.83784440	-12.1902	-199.30271523	-21.0303	-293.2141	-10.3432	
1.754					-198.83346368	-9.4413	-198.83440123	-198.83562583	-10.7981	-199.29910407	-18.7642	-292.1938	-9.3229	
1.774					-198.83250760	-8.8414	-198.83339577	-198.83455806	-10.1280	-199.29737254	-17.6777	-291.7072	-8.8363	
1.794					-198.83158196	-8.2605	-198.83242252	-198.83352431	-9.4793	-199.29569811	-16.6269	-291.2373	-8.3664	
1.814					-198.83069009	-7.7009	-198.83148484	-198.83252807	-8.8542	-199.29408499	-15.6147	-290.7847	-7.9138	
1.834					-198.82983444	-7.1639	-198.83058523	-198.83157192	-8.2542	-199.29253630	-14.6429	-290.3499	-7.4789	
1.854					-198.82901675	-6.6508	-198.82972542	-198.83065766	-7.6805	-199.29105417	-13.7128	-289.9329	-7.0620	
1.874					-198.82823810	-6.1622	-198.82890650	-198.82978642	-7.1338	-199.28963987	-12.8253	-289.5340	-6.6631	
1.894					-198.82749906	-5.6985	-198.82812899	-198.82895877	-6.6144	-199.28829393	-11.9808	-289.1532	-6.2823	
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1.954					-198.82551843	-4.4556	-198.82604363	-198.82673595	-5.2196	-199.28466237	-9.7019	-288.1172	-5.2463	
1.974					-198.82493502	-4.0895	-198.82542872	-198.82607950	-4.8077	-199.28358356	-9.0249	-287.8064	-4.9355	
1.994					-198.82438837	-3.7465	-198.82485219	-198.82546351	-4.4211	-199.28256781	-8.3876	-287.5120	-4.6411	
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2.034					-198.82340017	-3.1264	-198.82380886	-198.82434730	-3.7207	-199.28071703	-7.2262	-286.9707	-4.0998	
2.054					-198.82295576	-2.8475	-198.82333910	-198.82384400	-3.4049	-199.27987732	-6.6992	-286.7227	-3.8518	
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2.194					-198.82062943	-1.3877	-198.82087087	-198.82118892	-1.7388	-199.27536423	-3.8672	-285.3505	-2.4795	
2.214					-198.82039103	-1.2381	-198.82061659	-198.82091393	-1.5662	-199.27488457	-3.5663	-285.1991	-2.3281	
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2.254	-198.81997064	-0.9743	-198.82016722	-198.82042693	-1.2606	-199.27402574	-3.0273	-284.9239	-2.0530
2.274	-198.81978615	-0.8585	-198.81996954	-198.82021218	-1.1259	-199.27364238	-2.7868	-284.7991	-1.9282
2.294	-198.81961724	-0.7525	-198.81978823	-198.82001489	-1.0021	-199.27328709	-2.5638	-284.6822	-1.8113
2.314	-198.81946281	-0.6556	-198.81962216	-198.81983386	-0.8885	-199.27295802	-2.3573	-284.5726	-1.7017
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2.354	-198.81919329	-0.4865	-198.81933149	-198.81951610	-0.6891	-199.27237163	-1.9894	-284.3738	-1.5028
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2.394	-198.81897003	-0.3464	-198.81908967	-198.81925059	-0.5225	-199.27187035	-1.6748	-284.1993	-1.3284
2.444	-198.81874588	-0.2058	-198.81884554	-198.81898105	-0.3533	-199.27134615	-1.3459	-284.0110	-1.1401
2.494	-198.81857232	-0.0968	-198.81865514	-198.81876922	-0.2204	-199.27091780	-1.0771	-283.8511	-0.9802
2.544	-198.81843980	-0.0137	-198.81850848	-198.81860453	-0.1170	-199.27056885	-0.8581	-283.7153	-0.8444
2.594	-198.81834031	0.0487	-198.81839717	-198.81847806	-0.0377	-199.27028538	-0.6802	-283.5999	-0.7290
2.644	-198.81826718	0.0946	-198.81831418	-198.81838233	0.0224	-199.27005570	-0.5361	-283.5016	-0.6307
2.694	-198.81821486	0.1275	-198.81825368	-198.81831113	0.0671	-199.26987004	-0.4196	-283.4180	-0.5471
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2.844	-198.81814154	0.1735	-198.81816336	-198.81819799	0.1381	-199.26950280	-0.1891	-283.2335	-0.3626
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3.094	-198.81815040	0.1679	-198.81815880	-198.81817419	0.1530	-199.26924241	-0.0257	-283.0646	-0.1937
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3.494	-198.81823632	0.1140	-198.81823827	-198.81824314	0.1097	-199.26915238	0.0308	-282.9542	-0.0832
3.544	-198.81824682	0.1074	-198.81824845	-198.81825273	0.1037	-199.26915107	0.0316	-282.9467	-0.0758
3.594	-198.81825691	0.1011	-198.81825828	-198.81826206	0.0979	-199.26915068	0.0318	-282.9402	-0.0693
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3.694	-198.81827575	0.0893	-198.81827673	-198.81827972	0.0868	-199.26915178	0.0311	-282.9290	-0.0581
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3.994	-198.81832058	0.0611	-198.81832095	-198.81832255	0.0599	-199.26916101	0.0253	-282.9067	-0.0358
4.044	-198.81832642	0.0575	-198.81832674	-198.81832820	0.0561	-199.26916267	0.0243	-282.9041	-0.0332
4.094	-198.81833185	0.0541	-198.81833213	-198.81833345	0.0531	-199.26916429	0.0233	-282.9017	-0.0308
4.144	-198.81833689	0.0509	-198.81833713	-198.81833835	0.0500	-199.26916585	0.0223	-282.8995	-0.0286
4.194	-198.81834157	0.0480	-198.81834178	-198.81834290	0.0471	-199.26916734	0.0214	-282.8975	-0.0266
4.244	-198.81834592	0.0452	-198.81834610	-198.81834713	0.0445	-199.26916876	0.0205	-282.8957	-0.0247
4.294	-198.81834996	0.0427	-198.81835012	-198.81835102	0.0420	-199.26917012	0.0196	-282.8940	-0.0231
4.344	-198.81835372	0.0403	-198.81835386	-198.81835474	0.0397	-199.26917141	0.0188	-282.8924	-0.0215
4.394	-198.81835722	0.0381	-198.81835734	-198.81835815	0.0376	-199.26917264	0.0180	-282.8910	-0.0201
4.444	-198.81836048	0.0361	-198.81836059	-198.81836134	0.0356	-199.26917381	0.0173	-282.8897	-0.0188
4.494	-198.81836352	0.0342	-198.81836361	-198.81836431	0.0337	-199.26917493	0.0166	-282.8885	-0.0176
4.544	-198.81836636	0.0324	-198.81836644	-198.81836709	0.0320	-199.26917599	0.0159	-282.8874	-0.0165
4.594	-198.81836901	0.0307	-198.81836909	-198.81836969	0.0303	-199.26917701	0.0153	-282.8863	-0.0154
4.644	-198.81837150	0.0292	-198.81837156	-198.81837213	0.0288	-199.26917798	0.0147	-282.8854	-0.0145
4.694	-198.81837383	0.0277	-198.81837388	-198.81837441	0.0274	-199.26917891	0.0141	-282.8845	-0.0136
4.744	-198.81837601	0.0263	-198.81837606	-198.81837656	0.0260	-199.26917979	0.0136	-282.8837	-0.0128
4.794	-198.81837806	0.0251	-198.81837811	-198.81837857	0.0247	-199.26918065	0.0130	-282.8830	-0.0120
4.844	-198.81837998	0.0239	-198.81838003	-198.81838046	0.0236	-199.26918146	0.0125	-282.8823	-0.0113
4.894	-198.81838179	0.0227	-198.81838183	-198.81838224	0.0224	-199.26918225	0.0120	-282.8816	-0.0107
4.944	-198.81838510	0.0206	-198.81838513	-198.81838549	0.0204	-199.26918372	0.0111	-282.8805	-0.0096
5.094	-198.81838804	0.0188	-198.81838807	-198.81838839	0.0186	-199.26918508	0.0102	-282.8795	-0.0086
5.194	-198.81839066	0.0171	-198.81839068	-198.81839096	0.0170	-199.26918635	0.0094	-282.8786	-0.0077
5.294	-198.81839300	0.0157	-198.81839302	-198.81839327	0.0155	-199.26918753	0.0087	-282.8779	-0.0070
5.394	-198.81839509	0.0144	-198.81839511	-198.81839534	0.0142	-199.26918863	0.0080	-282.8773	-0.0064
5.494	-198.81839698	0.0132	-198.81839699	-198.81839720	0.0131	-199.26918967	0.0074	-282.8767	-0.0058
5.594	-198.81839868	0.0121	-198.81839869	-198.81839887	0.0120	-199.26919064	0.0067	-282.8763	-0.0054
5.694	-198.81840022	0.0112	-198.81840023	-198.81840039	0.0111	-199.26919157	0.0062	-282.8759	-0.0050
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5.894	-198.81840289	0.0095	-198.81840290	-198.81840303	0.0094	-199.26919328	0.0051	-282.8753	-0.0044
5.994	-198.81840404	0.0088	-198.81840406	-198.81840417	0.0087	-199.26919408	0.0046	-282.8751	-0.0042
6.094	-198.81840510	0.0081	-198.81840511	-198.81840522	0.0080	-199.26919484	0.0041	-282.8749	-0.0040
6.194	-198.81840607	0.0075	-198.81840608	-198.81840618	0.0074	-199.26919556	0.0037	-282.8747	-0.0038
6.294	-198.81840696	0.0069	-198.81840697	-198.81840705	0.0069	-199.26919625	0.0032	-282.8746	-0.0037
6.394	-198.81840778	0.0064	-198.81840778	-198.81840786	0.0064	-199.26919691	0.0028	-282.8745	-0.0036
6.494	-198.81840852	0.0059	-198.81840852	-198.81840860	0.0059	-199.26919754	0.0024	-282.8744	-0.0035

6.594		-198.81840920	0.0055	-198.81840921	-198.81840927	0.0055	-199.26919813	0.0020	-282.8744	-0.0035
6.694		-198.81840983	0.0051	-198.81840983	-198.81840989	0.0051	-199.26919870	0.0017	-282.8743	-0.0034
6.794		-198.81841041	0.0048	-198.81841041	-198.81841047	0.0047	-199.26919924	0.0013	-282.8743	-0.0034
6.894		-198.81841094	0.0044	-198.81841094	-198.81841099	0.0044	-199.26919976	0.0010	-282.8743	-0.0034
6.994		-198.81841143	0.0041	-198.81841143	-198.81841148	0.0041	-199.26920025	0.0007	-282.8743	-0.0034
7.094		-198.81841188	0.0038	-198.81841188	-198.81841192	0.0038	-199.26920071	0.0004	-282.8743	-0.0034
7.194		-198.81841229	0.0036	-198.81841229	-198.81841233	0.0036	-199.26920116	0.0001	-282.8743	-0.0034
7.294		-198.81841267	0.0033	-198.81841267	-198.81841271	0.0033	-199.26920158	-0.0001	-282.8744	-0.0035
7.394		-198.81841302	0.0031	-198.81841302	-198.81841306	0.0031	-199.26920198	-0.0004	-282.8744	-0.0035
7.494		-198.81841335	0.0029	-198.81841335	-198.81841338	0.0029	-199.26920237	-0.0006	-282.8744	-0.0035
7.594		-198.81841365	0.0027	-198.81841365	-198.81841368	0.0027	-199.26920273	-0.0008	-282.8745	-0.0036
7.694		-198.81841393	0.0025	-198.81841393	-198.81841395	0.0025	-199.26920308	-0.0011	-282.8745	-0.0036
7.794		-198.81841418	0.0024	-198.81841418	-198.81841421	0.0024	-199.26920341	-0.0013	-282.8746	-0.0037
7.894		-198.81841442	0.0022	-198.81841442	-198.81841444	0.0022	-199.26920373	-0.0015	-282.8746	-0.0037
7.994		-198.81841464	0.0021	-198.81841464	-198.81841466	0.0021	-199.26920404	-0.0017	-282.8747	-0.0038
8.094		-198.81841483	0.0020	-198.81841485	-198.81841487	0.0020	-199.26920433	-0.0018	-282.8747	-0.0038
8.194		-198.81841502	0.0019	-198.81841504	-198.81841506	0.0019	-199.26920460	-0.0020	-282.8748	-0.0039
8.294		-198.81841520	0.0018	-198.81841521	-198.81841523	0.0017	-199.26920487	-0.0022	-282.8748	-0.0039
8.394		-198.81841536	0.0017	-198.81841538	-198.81841539	0.0016	-199.26920512	-0.0023	-282.8749	-0.0040
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8.694		-198.81841579	0.0014	-198.81841581	-198.81841582	0.0014	-199.26920582	-0.0028	-282.8751	-0.0042
8.794		-198.81841591	0.0013	-198.81841593	-198.81841594	0.0013	-199.26920604	-0.0029	-282.8751	-0.0042
8.894		-198.81841603	0.0012	-198.81841605	-198.81841606	0.0012	-199.26920625	-0.0030	-282.8752	-0.0043
8.994		-198.81841614	0.0012	-198.81841615	-198.81841617	0.0012	-199.26920644	-0.0032	-282.8752	-0.0043
9.094		-198.81841624	0.0011	-198.81841626	-198.81841627	0.0011	-199.26919989	0.0009	-282.8711	-0.0002
9.194		-198.81841633	0.0010	-198.81841635	-198.81841636	0.0010	-199.26919997	0.0009	-282.8711	-0.0002
9.294		-198.81841642	0.0010	-198.81841644	-198.81841645	0.0010	-199.26920004	0.0008	-282.8710	-0.0001
9.394		-198.81841651	0.0009	-198.81841652	-198.81841653	0.0009	-199.26920011	0.0008	-282.8710	-0.0001
9.494		-198.81841658	0.0009	-198.81841660	-198.81841661	0.0009	-199.26920018	0.0008	-282.8710	-0.0001
9.594		-198.81841666	0.0008	-198.81841667	-198.81841668	0.0008	-199.26920024	0.0007	-282.8710	-0.0001
9.694		-198.81841673	0.0008	-198.81841674	-198.81841675	0.0008	-199.26920029	0.0007	-282.8710	-0.0001
9.794		-198.81841679	0.0008	-198.81841681	-198.81841681	0.0008	-199.26920035	0.0007	-282.8710	-0.0001
9.894		-198.81841685	0.0007	-198.81841687	-198.81841688	0.0007	-199.26920040	0.0006	-282.8710	-0.0001
20.000		-198.81841799	0.0000	-198.81841801	-198.81841801	0.0000	-199.26920139	0.0000	-282.8709	0.0000

Re		
1.415		
DCE (Re-shifted)		
AR	vCASC13-SCGVB	Δ(vCASC13-SCGVB)
-0.331	-306.7586	-23.8876
-0.321	-306.7043	-23.8334
-0.311	-306.6464	-23.7755
-0.301	-306.5844	-23.7135
-0.291	-306.5178	-23.6469
-0.281	-306.4461	-23.5752
-0.271	-306.3689	-23.4980
-0.261	-306.2859	-23.4150
-0.251	-306.1967	-23.3258
-0.241	-306.1010	-23.2301
-0.231	-305.9985	-23.1276
-0.221	-305.8891	-23.0182
-0.211	-305.7725	-22.9016
-0.201	-305.6486	-22.7777
-0.191	-305.5173	-22.6464
-0.181	-305.3786	-22.5076
-0.161	-305.0784	-22.2074
-0.141	-304.7480	-21.8771
-0.121	-304.3879	-21.5170
-0.101	-303.9990	-21.1281
-0.081	-303.5823	-20.7113
-0.061	-303.1393	-20.2684
-0.041	-302.6718	-19.8009
-0.021	-302.1819	-19.3109
-0.001	-301.6715	-18.8006
0.019	-301.1431	-18.2722
0.039	-300.5991	-17.7282
0.059	-300.0419	-17.1710
0.079	-299.4741	-16.6032
0.099	-298.8983	-16.0274
0.119	-298.3170	-15.4460
0.139	-297.7326	-14.8617
0.159	-297.1476	-14.2767
0.179	-296.5643	-13.6934
0.199	-295.9849	-13.1140
0.219	-295.4115	-12.5406
0.239	-294.8460	-11.9751
0.259	-294.2903	-11.4194
0.279	-293.7458	-10.8749
0.299	-293.2141	-10.3432
0.339	-292.1938	-9.3229
0.359	-291.7072	-8.8363
0.379	-291.2373	-8.3664
0.399	-290.7847	-7.9138
0.419	-290.3499	-7.4789
0.439	-289.9329	-7.0620
0.459	-289.5340	-6.6631
0.479	-289.1532	-6.2823
0.499	-288.7903	-5.9194
0.519	-288.4451	-5.5742
0.539	-288.1172	-5.2463
0.559	-287.8064	-4.9355
0.579	-287.5120	-4.6411
0.599	-287.2336	-4.3627
0.619	-286.9707	-4.0998
0.639	-286.7227	-3.8518
0.659	-286.4889	-3.6180
0.679	-286.2687	-3.3978
0.699	-286.0615	-3.1906
0.719	-285.8667	-2.9958
0.739	-285.6837	-2.8128
0.759	-285.5118	-2.6409
0.779	-285.3505	-2.4795
0.799	-285.1991	-2.3281
0.819	-285.0571	-2.1862

0.839	-284.9239	-2.0530
0.859	-284.7991	-1.9282
0.879	-284.6822	-1.8113
0.899	-284.5726	-1.7017
0.919	-284.4699	-1.5990
0.939	-284.3738	-1.5028
0.959	-284.2837	-1.4128
0.979	-284.1993	-1.3284
1.029	-284.0110	-1.1401
1.079	-283.8511	-0.9802
1.129	-283.7153	-0.8444
1.179	-283.5999	-0.7290
1.229	-283.5016	-0.6307
1.279	-283.4180	-0.5471
1.329	-283.3466	-0.4757
1.379	-283.2857	-0.4147
1.429	-283.2335	-0.3626
1.479	-283.1888	-0.3179
1.529	-283.1505	-0.2796
1.579	-283.1175	-0.2466
1.629	-283.0891	-0.2182
1.679	-283.0646	-0.1937
1.729	-283.0433	-0.1724
1.779	-283.0249	-0.1540
1.829	-283.0089	-0.1380
1.879	-282.9949	-0.1240
1.929	-282.9827	-0.1118
1.979	-282.9719	-0.1010
2.029	-282.9625	-0.0916
2.079	-282.9542	-0.0832
2.129	-282.9467	-0.0758
2.179	-282.9402	-0.0693
2.229	-282.9343	-0.0634
2.279	-282.9290	-0.0581
2.329	-282.9243	-0.0534
2.379	-282.9201	-0.0491
2.429	-282.9162	-0.0453
2.479	-282.9127	-0.0418
2.529	-282.9096	-0.0387
2.579	-282.9067	-0.0358
2.629	-282.9041	-0.0332
2.679	-282.9017	-0.0308
2.729	-282.8995	-0.0286
2.779	-282.8975	-0.0266
2.829	-282.8957	-0.0247
2.879	-282.8940	-0.0231
2.929	-282.8924	-0.0215
2.979	-282.8910	-0.0201
3.029	-282.8897	-0.0188
3.079	-282.8885	-0.0176
3.129	-282.8874	-0.0165
3.179	-282.8863	-0.0154
3.229	-282.8854	-0.0145
3.279	-282.8845	-0.0136
3.329	-282.8837	-0.0128
3.379	-282.8830	-0.0120
3.429	-282.8823	-0.0113
3.479	-282.8816	-0.0107
3.579	-282.8805	-0.0096
3.679	-282.8795	-0.0086
3.779	-282.8786	-0.0077
3.879	-282.8779	-0.0070
3.979	-282.8773	-0.0064
4.079	-282.8767	-0.0058
4.179	-282.8763	-0.0054
4.279	-282.8759	-0.0050
4.379	-282.8756	-0.0047
4.479	-282.8753	-0.0044
4.579	-282.8751	-0.0042
4.679	-282.8749	-0.0040
4.779	-282.8747	-0.0038
4.879	-282.8746	-0.0037
4.979	-282.8745	-0.0036
5.079	-282.8744	-0.0035

5.179	-282.8744	-0.0035
5.279	-282.8743	-0.0034
5.379	-282.8743	-0.0034
5.479	-282.8743	-0.0034
5.579	-282.8743	-0.0034
5.679	-282.8743	-0.0034
5.779	-282.8743	-0.0034
5.879	-282.8744	-0.0035
5.979	-282.8744	-0.0035
6.079	-282.8744	-0.0035
6.179	-282.8745	-0.0036
6.279	-282.8745	-0.0036
6.379	-282.8746	-0.0037
6.479	-282.8746	-0.0037
6.579	-282.8747	-0.0038
6.679	-282.8747	-0.0038
6.779	-282.8748	-0.0039
6.879	-282.8748	-0.0039
6.979	-282.8749	-0.0040
7.079	-282.8750	-0.0041
7.179	-282.8750	-0.0041
7.279	-282.8751	-0.0042
7.379	-282.8751	-0.0042
7.479	-282.8752	-0.0043
7.579	-282.8752	-0.0043
7.679	-282.8711	-0.0002
7.779	-282.8711	-0.0002
7.879	-282.8710	-0.0001
7.979	-282.8710	-0.0001
8.079	-282.8710	-0.0001
8.179	-282.8710	-0.0001
8.279	-282.8710	-0.0001
8.379	-282.8710	-0.0001
8.479	-282.8710	-0.0001
18.585	-282.8709	0.0000