

Electronic Supplementary Information

Effect of π - π interaction in Bergman Cyclization

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1. SI for SAPT and EDA

The interaction energy calculated using BP86 functional. All the energies are in kcal/mol.

Table1 $R_1 = R_2 = \text{Ph}$

Entry	IE_DFT	SAPT2+3	SAPT2+(3)	SAPT2+	SAPT2	SAPT0
1	-3.89446534	-4.02221849	-3.79542811	-4.32600346	-6.11558978	-5.66869057
2	-3.80123335	-4.11616631	-3.91784175	-4.40558973	-6.05496659	-5.62551819
3	-3.606678	-4.09076178	-3.90428953	-4.36436361	-5.90713735	-5.48975544
4	-3.35251263	-3.99529738	-3.80968571	-4.2538805	-5.71610015	-5.30608582
5	-3.07127909	-3.85631253	-3.66405607	-4.1014647	-5.50326934	-5.09753096
6	-2.88622565	-3.82918438	-3.64841792	-4.06174452	-5.3543318	-4.95711402
7	-2.71010162	-3.79263617	-3.62114381	-4.01525757	-5.21282806	-4.8231893
8	-2.54939017	-3.72981286	-3.56436528	-3.94327473	-5.0602222	-4.68152181
9	-2.41182568	-3.6489887	-3.48805958	-3.85384902	-4.89958899	-4.53573441
10	-2.30019895	-3.54514758	-3.38676096	-3.74112806	-4.72522834	-4.38162795
11	-2.20652056	-3.43051188	-3.27405612	-3.61815017	-4.54675399	-4.22702772
12	-1.90671043	-2.82948242	-2.60851325	-3.00763282	-4.02050764	-3.73844389
13	-1.46579673	-2.10782973	-1.79252685	-2.26737011	-3.39525272	-3.15539202
14	-0.85586944	-1.31272917	-0.88715688	-1.44704373	-2.67149654	-2.46517657
15	-0.03380447	-0.42122167	0.11512846	-0.52754148	-1.77240862	-1.6046412
16	1.48816373	1.09200212	1.80126597	1.03978795	-0.2151072	-0.09217162
17	1.59033426	1.32903382	2.04007777	1.27879889	0.08451243	0.15179745

Table2 $R_1 = R_2 = \text{Ph}$

Entry	IE_DFT	SAPT2+3	Exchange	Electrostatic	Induction	Dispersion
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1	-3.89446534	-4.02221849	8.65799143	-3.87255753	-0.92002108	-7.88763132
2	-3.80123335	-4.11616631	7.74113824	-3.66885215	-0.85017567	-7.33827673
3	-3.606678	-4.09076178	7.25195355	-3.60393369	-0.80981927	-6.92896237
4	-3.35251263	-3.99529738	7.06602499	-3.63799819	-0.79135469	-6.6319695
5	-3.07127909	-3.85631253	7.09749587	-3.73698893	-0.79002746	-6.42679202
6	-2.88622565	-3.82918438	6.68429522	-3.73456313	-0.74453574	-6.03438072
7	-2.71010162	-3.79263617	6.3571176	-3.73874574	-0.70913697	-5.70187105
8	-2.54939017	-3.72981286	6.12665238	-3.74280219	-0.6844007	-5.42926235
9	-2.41182568	-3.6489887	5.9446834	-3.72843976	-0.66647902	-5.19875331
10	-2.30019895	-3.54514758	5.81604668	-3.69546094	-0.65586184	-5.00987148
11	-2.20652056	-3.43051188	5.70896088	-3.63565229	-0.65010772	-4.85371276
12	-1.90671043	-2.82948242	7.3306591	-3.96595764	-0.78504363	-5.40914024
13	-1.46579673	-2.10782973	9.59853435	-4.55365943	-0.97557663	-6.17712803
14	-0.85586944	-1.31272917	12.1777297	-5.27473965	-1.17868223	-7.03703696
15	-0.03380447	-0.42122167	14.8736412	-6.02313086	-1.3968657	-7.87486629
16	1.48816373	1.09200212	19.1368989	-7.17132277	-1.80289165	-9.07068235
17	1.59033426	1.32903382	19.3439033	-7.15659056	-1.81083673	-9.04744221

Table3 $R_1 = R_2 = \text{CH}_2\text{Ph}$

Entry	IE_DFT	SAPT2+3	SAPT2+(3)	SAPT2+	SAPT2	SAPT0
1	-1.42563641	-1.73744393	-1.64270878	-1.87614595	-2.35024364	-2.09515196
2	-1.53846943	-1.88794515	-1.79588997	-2.03402399	-2.55730616	-2.28464021
3	-1.6413453	-2.04899137	-1.9569141	-2.20417059	-2.78728801	-2.49108487
4	-1.76873225	-2.22905016	-2.13804096	-2.39341532	-3.03672735	-2.71866353
5	-1.91268023	-2.42594856	-2.33546808	-2.60046328	-3.30942077	-2.96874411
6	-2.07374957	-2.64080393	-2.54996845	-2.82671954	-3.60839802	-3.24442966
7	-2.2512719	-2.8734994	-2.78084226	-3.07237133	-3.93621008	-3.54858617
8	-2.45601406	-3.12153459	-3.02519921	-3.33449228	-4.28898019	-3.88027916
9	-2.66139603	-3.37225108	-3.26689279	-3.6031915	-4.67710002	-4.24065507
10	-2.91183075	-3.58970023	-3.47501624	-3.83612479	-5.01795711	-4.56707603
11	-3.18746649	-3.78521338	-3.64938108	-4.05211213	-5.39974264	-4.93432518
12	-3.44813228	-3.87192702	-3.69908748	-4.15828422	-5.71068588	-5.24051728
13	-3.60570367	-3.73768802	-3.49981036	-4.03746874	-5.8436076	-5.38587398
14	-3.55186285	-3.40070462	-3.07812375	-3.69868774	-5.73798836	-5.30086287
15	-3.5537309	-3.43197324	-3.10540398	-3.72302009	-5.73280131	-5.29611615
16	-3.54199105	-3.45924917	-3.13015923	-3.75216355	-5.77613559	-5.32899845
17	-3.21680485	-2.70937165	-2.24679828	-2.98540673	-5.30751518	-4.89856403

Table4 $R_1 = R_2 = \text{CH}_2\text{Ph}$

Entry	IE_DFT	SAPT2+3	Exchange	Electrostatic	Induction	Dispersion
1	-1.42563641	-1.73744393	3.57047117	-1.26977485	-0.41529536	-3.62284489
2	-1.53846943	-1.88794515	3.57543398	-1.34511343	-0.41340921	-3.7048565
3	-1.6413453	-2.04899137	3.65969774	-1.44247067	-0.42409342	-3.84212501
4	-1.76873225	-2.22905016	3.71923349	-1.54002046	-0.43147845	-3.97678475
5	-1.91268023	-2.42594856	3.80344552	-1.65003128	-0.44220307	-4.13715974
6	-2.07374957	-2.64080393	3.92512797	-1.77776137	-0.45738402	-4.33078651
7	-2.2512719	-2.8734994	4.10312067	-1.92994143	-0.4785891	-4.56808954

8	-2.45601406	-3.12153459	4.34293842	-2.11183398	-0.50429965	-4.84833938
9	-2.66139603	-3.37225108	4.76311409	-2.34816692	-0.55189591	-5.23530234
10	-2.91183075	-3.58970023	5.16472507	-2.56365758	-0.58831938	-5.60244834
11	-3.18746649	-3.78521338	5.9369429	-2.87759799	-0.66100999	-6.1835483
12	-3.44813228	-3.87192702	7.108003	-3.28145462	-0.76505301	-6.93342239
13	-3.60570367	-3.73768802	8.94639423	-3.84582628	-0.92192646	-7.91632951
14	-3.55186285	-3.40070462	11.1256392	-4.53649736	-1.10419609	-8.88565034
15	-3.5537309	-3.43197324	11.1232096	-4.6178873	-1.10066684	-8.83662866
16	-3.54199105	-3.45924917	11.2068901	-4.66599706	-1.11509955	-8.8850427
17	-3.21680485	-2.70937165	14.5282713	-5.66598564	-1.38617871	-10.1854786

Table5 $R_1 = \text{CH}_2\text{CH}_2\text{Ph}$, $R_2 = \text{CH}_2\text{Ph}$

Entry	IE_DFT	SAPT2+3	SAPT2+(3)	SAPT2+	SAPT2	SAPT0
1	-1.75125736	-0.14672246	0.7660778	-0.33600306	-3.64542063	-3.326751
2	-2.57745279	-1.31574289	-0.64832891	-1.57652942	-4.44922991	-4.03644136
3	-2.87765985	-1.99644007	-1.48218854	-2.29154581	-4.8664582	-4.35669541
4	-3.19674367	-2.63445822	-2.22399204	-2.94232078	-5.25521569	-4.73498222
5	-3.26820836	-2.83556315	-2.45739529	-3.14212675	-5.35369873	-4.84104838
6	-3.40518397	-3.16610003	-2.86360493	-3.4736586	-5.47586443	-4.96264397
7	-3.46697149	-3.39379849	-3.14173083	-3.69569498	-5.53699341	-5.04673786
8	-3.58165549	-3.58051212	-3.35950763	-3.87146185	-5.57270042	-5.14422763
9	-3.6050178	-3.75620803	-3.55333369	-4.03847773	-5.64475609	-5.26129302
10	-3.60659165	-3.93185352	-3.7418396	-4.20619929	-5.73189937	-5.38060149
11	-3.53000773	-4.0114729	-3.81573367	-4.27608369	-5.75191901	-5.43953932
12	-3.44490788	-4.09045058	-3.89841113	-4.34288957	-5.74118106	-5.46203168
13	-3.34680749	-4.07520763	-3.87544343	-4.31302671	-5.65664376	-5.41900463
14	-3.22385929	-3.9800944	-3.76156307	-4.20140634	-5.51383095	-5.32213715
15	-3.08639226	-3.83892797	-3.59081823	-4.0443152	-5.3580811	-5.20567414
16	-2.99999129	-3.77591497	-3.5130049	-3.96892042	-5.2566869	-5.13131466
17	-2.91163196	-3.70409765	-3.42918231	-3.88808838	-5.15978297	-5.05131541

Table6 $R_1 = \text{CH}_2\text{CH}_2\text{Ph}$, $R_2 = \text{CH}_2\text{Ph}$

Entry	IE_DFT	SAPT2+3	Exchange	Electrostatic	Induction	Dispersion
1	-1.75125736	-0.14672246	25.6858343	-9.38265997	-2.3159593	-14.1339375
2	-2.57745279	-1.31574289	20.0347932	-7.26208165	-1.76440747	-12.324047
3	-2.87765985	-1.99644007	16.4126913	-5.9657043	-1.40977001	-11.0336571
4	-3.19674367	-2.63445822	13.7754373	-5.19626867	-1.20099624	-10.0126306
5	-3.26820836	-2.83556315	12.8400332	-4.91807102	-1.15579569	-9.60172958
6	-3.40518397	-3.16610003	10.8546812	-4.25219518	-1.01424213	-8.75434389
7	-3.46697149	-3.39379849	9.43662064	-3.77790311	-0.93925988	-8.11325614
8	-3.58165549	-3.58051212	8.44416533	-3.50978439	-0.89164228	-7.62325078
9	-3.6050178	-3.75620803	7.83082335	-3.43750352	-0.869603	-7.27992485
10	-3.60659165	-3.93185352	7.3931466	-3.48813764	-0.83859102	-6.99827145
11	-3.53000773	-4.0114729	7.43575908	-3.72626528	-0.84240285	-6.87856384
12	-3.44490788	-4.09045058	7.21681622	-3.87363575	-0.81199333	-6.62163772
13	-3.34680749	-4.07520763	7.27419305	-4.06841102	-0.80630822	-6.47468144
14	-3.22385929	-3.9800944	7.59488632	-4.30696749	-0.82878708	-6.43922614
15	-3.08639226	-3.83892797	8.20160769	-4.62023419	-0.87827178	-6.54202968

16	-2.99999129	-3.77591497	8.47057491	-4.81079029	-0.90175138	-6.5339482
17	-2.91163196	-3.70409765	8.71121232	-4.95248381	-0.92419507	-6.53863109

Table7 $R_1 = R_2 = \text{CH}_2\text{CH}_2\text{Ph}$

Entry	IE_DFT	SAPT2+3	SAPT2+(3)	SAPT2+	SAPT2	SAPT0
1	-3.83836581	-3.79927872	-3.46728467	-4.07574657	-6.02909238	-5.73695326
2	-3.89849348	-3.79375299	-3.47180045	-4.07596355	-6.02376592	-5.72058347
3	-3.90701898	-3.76719191	-3.45386059	-4.05553454	-6.006651	-5.68222636
4	-3.86366824	-3.72169147	-3.41567973	-4.01666851	-5.9799931	-5.62436455
5	-3.83499275	-3.68772848	-3.39100437	-3.98336035	-5.92216059	-5.54435674
6	-3.76398414	-3.66709607	-3.38750715	-3.96473705	-5.86720567	-5.45903228
7	-3.68900041	-3.66051509	-3.40256502	-3.95690512	-5.79273949	-5.35985982
8	-3.62316997	-3.68916192	-3.4563627	-3.98247217	-5.73008474	-5.27617806
9	-3.50653508	-3.72480708	-3.51429751	-4.01539677	-5.68916175	-5.20516451
10	-3.47658032	-3.76504432	-3.56187396	-4.05568736	-5.70846258	-5.21237909
11	-3.42170552	-3.82351858	-3.63215101	-4.11228855	-5.72216562	-5.21071834
12	-3.48110389	-3.86907229	-3.67243488	-4.15905438	-5.79142886	-5.29698636
13	-3.37438936	-3.96722727	-3.79138299	-4.24960119	-5.78465542	-5.26579515
14	-3.35746321	-4.04140715	-3.87414027	-4.32036964	-5.81363041	-5.29435809
15	-3.39121019	-4.06718937	-3.89845903	-4.3444641	-5.83913658	-5.34128174
16	-3.47567213	-4.10772796	-3.93783852	-4.37926306	-5.85372461	-5.39805721
17	-3.52676454	-4.11485548	-3.93678134	-4.38282701	-5.8647879	-5.44952062

Table8 $R_1 = R_2 = \text{CH}_2\text{CH}_2\text{Ph}$

Entry	IE_DFT	SAPT2+3	Exchange	Electrostatic	Induction	Dispersion
1	-3.83836581	-3.79927872	11.0702374	-4.98349698	-1.17303369	-8.71298541
2	-3.89849348	-3.79375299	10.8800627	-4.82251774	-1.15366937	-8.69762862
3	-3.90701898	-3.76719191	10.7395604	-4.67804549	-1.13601647	-8.69269039
4	-3.86366824	-3.72169147	10.646787	-4.55100188	-1.11907936	-8.69839721
5	-3.83499275	-3.68772848	10.4153146	-4.41591852	-1.08911088	-8.59801365
6	-3.76398414	-3.66709607	10.0277436	-4.22411911	-1.04745788	-8.42326263
7	-3.68900041	-3.66051509	9.46587119	-3.99601796	-0.98574569	-8.14462263
8	-3.62316997	-3.68916192	8.77342864	-3.76190616	-0.90774916	-7.79293524
9	-3.50653508	-3.72480708	8.16668888	-3.58470908	-0.84234271	-7.46444416
10	-3.47658032	-3.76504432	7.96894435	-3.54639106	-0.82006238	-7.36753524
11	-3.42170552	-3.82351858	7.62651544	-3.48586918	-0.78376597	-7.18039888
12	-3.48110389	-3.86907229	7.74513648	-3.55026893	-0.80398464	-7.2599552
13	-3.37438936	-3.96722727	7.11226465	-3.46061491	-0.73902694	-6.87985007
14	-3.35746321	-4.04140715	6.83401119	-3.43558513	-0.71899193	-6.72084128
15	-3.39121019	-4.06718937	6.83453381	-3.45108305	-0.73538635	-6.71525378
16	-3.47567213	-4.10772796	6.77996009	-3.47157813	-0.74880654	-6.66730338
17	-3.52676454	-4.11485548	6.94774834	-3.55774099	-0.78605684	-6.718806

Table9 $R_1 = R_2 = \text{CH}_2\text{OPh}$

Entry	IE_DFT	SAPT2+3	SAPT2+(3)	SAPT2+	SAPT2	SAPT0
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1	-2.96924022	-3.76315024	-3.4690183	-3.9748786	-5.4617276	-5.20141695
2	-3.14776358	-3.85114752	-3.56003821	-4.07398067	-5.61176542	-5.34357928
3	-3.31566029	-3.89501922	-3.60461089	-4.1285715	-5.72607672	-5.45268301
4	-3.46489906	-3.89760443	-3.60539053	-4.1414551	-5.80435146	-5.52677365
5	-3.58133671	-3.86401765	-3.56644562	-4.11804968	-5.8552255	-5.5710777
6	-3.64545911	-3.79078979	-3.48245124	-4.0554776	-5.8856141	-5.58819179
7	-3.73839833	-3.78076263	-3.47748838	-4.05337765	-5.90869276	-5.6030915
8	-3.77783311	-3.73044341	-3.42650293	-4.0105231	-5.90515278	-5.58705155
9	-3.79548085	-3.66344557	-3.35449016	-3.94908079	-5.88362707	-5.55591682
10	-3.78890044	-3.59611015	-3.27696823	-3.88584073	-5.86549476	-5.52905817
11	-3.76094021	-3.55152865	-3.21667652	-3.84400487	-5.87581396	-5.53063844
12	-3.75456317	-3.51852345	-3.17471182	-3.81192775	-5.87067611	-5.5184089
13	-3.7085385	-3.43636216	-3.06933749	-3.72679712	-5.83842102	-5.48791478
14	-3.67553853	-3.32813367	-2.93718536	-3.6122595	-5.76533349	-5.42737727
15	-3.66268885	-3.2435674	-2.83732086	-3.52313738	-5.698353	-5.37208271
16	-3.56704294	-3.01358542	-2.56851684	-3.28113915	-5.51909807	-5.22081785
17	-3.62674654	-3.14376055	-2.72686131	-3.42066449	-5.61765862	-5.29209998

Table10 $R_1 = R_2 = \text{CH}_2\text{OPh}$

Entry	IE_DFT	SAPT2+3	Exchange	Electrostatic	Induction	Dispersion
1	-2.96924022	-3.76315024	9.68666247	-5.37996637	-0.99977954	-7.0700668
2	-3.14776358	-3.85114752	9.66734325	-5.27765828	-1.00208656	-7.23874592
3	-3.31566029	-3.89501922	9.70613943	-5.14818997	-1.01637553	-7.43659315
4	-3.46489906	-3.89760443	9.80998502	-5.00893039	-1.03986906	-7.65879
5	-3.58133671	-3.86401765	10.0111838	-4.888721	-1.07292643	-7.91355399
6	-3.64545911	-3.79078979	10.367074	-4.81628861	-1.11956331	-8.2220119
7	-3.73839833	-3.78076263	10.3031264	-4.66216905	-1.11209921	-8.30962072
8	-3.77783311	-3.73044341	10.3908592	-4.56849176	-1.11421335	-8.43859753
9	-3.79548085	-3.66344557	10.5764323	-4.5380301	-1.11958094	-8.58226685
10	-3.78890044	-3.59611015	10.880407	-4.58683754	-1.13492842	-8.75475117
11	-3.76094021	-3.55152865	11.3031334	-4.73115148	-1.16470284	-8.95880772
12	-3.75456317	-3.51852345	11.5467715	-4.80884041	-1.18030986	-9.07614462
13	-3.7085385	-3.43636216	12.1011467	-5.00932661	-1.23565017	-9.29253204
14	-3.67553853	-3.32813367	12.644086	-5.1906063	-1.29333789	-9.48827551
15	-3.66268885	-3.2435674	12.9928087	-5.29208468	-1.32964997	-9.61464148
16	-3.56704294	-3.01358542	13.8793174	-5.56748722	-1.41602361	-9.90939199
17	-3.62674654	-3.14376055	13.2462339	-5.32996152	-1.35433035	-9.70570259

The interaction energy calculated using B3LYP functional. All the energies are in kcal/mol.

Table11 $R_1 = R_2 = \text{Ph}$

Entry	IE_DFT	SAPT2+3	SAPT2+(3)	SAPT2+	SAPT2	SAPT0
1	-2.99610673	-4.02221849	-3.79542811	-4.32600346	-6.11558978	-5.66869057
2	-2.98966343	-4.11616631	-3.91784175	-4.40558973	-6.05496659	-5.62551819
3	-2.86566305	-4.09076178	-3.90428953	-4.36436361	-5.90713735	-5.48975544
4	-2.67271566	-3.99529738	-3.80968571	-4.2538805	-5.71610015	-5.30608582
5	-2.44218794	-3.85631253	-3.66405607	-4.1014647	-5.50326934	-5.09753096
6	-2.32720856	-3.82918438	-3.64841792	-4.06174452	-5.3543318	-4.95711402

7	-2.21235261	-3.79263617	-3.62114381	-4.01525757	-5.21282806	-4.8231893
8	-2.10300567	-3.72981286	-3.56436528	-3.94327473	-5.0602222	-4.68152181
9	-2.00927559	-3.6489887	-3.48805958	-3.85384902	-4.89958899	-4.53573441
10	-1.9328701	-3.54514758	-3.38676096	-3.74112806	-4.72522834	-4.38162795
11	-1.8713822	-3.43051188	-3.27405612	-3.61815017	-4.54675399	-4.22702772
12	-1.50901642	-2.82948242	-2.60851325	-3.00763282	-4.02050764	-3.73844389
13	-0.98325635	-2.10782973	-1.79252685	-2.26737011	-3.39525272	-3.15539202
14	-0.29735352	-1.31272917	-0.88715688	-1.44704373	-2.67149654	-2.46517657
15	0.59540068	-0.42122167	0.11512846	-0.52754148	-1.77240862	-1.6046412
16	2.27939753	1.09200212	1.80126597	1.03978795	-0.2151072	-0.09217162
17	2.36346194	1.32903382	2.04007777	1.27879889	0.08451243	0.15179745

Table12 $R_1 = R_2 = \text{Ph}$

Entry	IE_DFT	SAPT2+3	Exchange	Electrostatic	Induction	Dispersion
1	-2.99610673	-4.02221849	8.65799143	-3.87255753	-0.92002108	-7.88763132
2	-2.98966343	-4.11616631	7.74113824	-3.66885215	-0.85017567	-7.33827673
3	-2.86566305	-4.09076178	7.25195355	-3.60393369	-0.80981927	-6.92896237
4	-2.67271566	-3.99529738	7.06602499	-3.63799819	-0.79135469	-6.6319695
5	-2.44218794	-3.85631253	7.09749587	-3.73698893	-0.79002746	-6.42679202
6	-2.32720856	-3.82918438	6.68429522	-3.73456313	-0.74453574	-6.03438072
7	-2.21235261	-3.79263617	6.3571176	-3.73874574	-0.70913697	-5.70187105
8	-2.10300567	-3.72981286	6.12665238	-3.74280219	-0.6844007	-5.42926235
9	-2.00927559	-3.6489887	5.9446834	-3.72843976	-0.66647902	-5.19875331
10	-1.9328701	-3.54514758	5.81604668	-3.69546094	-0.65586184	-5.00987148
11	-1.8713822	-3.43051188	5.70896088	-3.63565229	-0.65010772	-4.85371276
12	-1.50901642	-2.82948242	7.3306591	-3.96595764	-0.78504363	-5.40914024
13	-0.98325635	-2.10782973	9.59853435	-4.55365943	-0.97557663	-6.17712803
14	-0.29735352	-1.31272917	12.1777297	-5.27473965	-1.17868223	-7.03703696
15	0.59540068	-0.42122167	14.8736412	-6.02313086	-1.3968657	-7.87486629
16	2.27939753	1.09200212	19.1368989	-7.17132277	-1.80289165	-9.07068235
17	2.36346194	1.32903382	19.3439033	-7.15659056	-1.81083673	-9.04744221

Table13 $R_1 = R_2 = \text{CH}_2\text{Ph}$

Entry	IE_DFT	SAPT2+3	SAPT2+(3)	SAPT2+	SAPT2	SAPT0
1	-1.32638541	-1.73744393	-1.64270878	-1.87614595	-2.35024364	-2.09515196
2	-1.41160036	-1.88794515	-1.79588997	-2.03402399	-2.55730616	-2.28464021
3	-1.48171938	-2.04899137	-1.9569141	-2.20417059	-2.78728801	-2.49108487
4	-1.5758587	-2.22905016	-2.13804096	-2.39341532	-3.03672735	-2.71866353
5	-1.68233203	-2.42594856	-2.33546808	-2.60046328	-3.30942077	-2.96874411
6	-1.80070243	-2.64080393	-2.54996845	-2.82671954	-3.60839802	-3.24442966
7	-1.92505643	-2.8734994	-2.78084226	-3.07237133	-3.93621008	-3.54858617
8	-2.0731202	-3.12153459	-3.02519921	-3.33449228	-4.28898019	-3.88027916
9	-2.20743374	-3.37225108	-3.26689279	-3.6031915	-4.67710002	-4.24065507
10	-2.38326725	-3.58970023	-3.47501624	-3.83612479	-5.01795711	-4.56707603
11	-2.55084945	-3.78521338	-3.64938108	-4.05211213	-5.39974264	-4.93432518
12	-2.67695576	-3.87192702	-3.69908748	-4.15828422	-5.71068588	-5.24051728
13	-2.68437449	-3.73768802	-3.49981036	-4.03746874	-5.8436076	-5.38587398

14	-2.50739875	-3.40070462	-3.07812375	-3.69868774	-5.73798836	-5.30086287
15	-2.52066567	-3.43197324	-3.10540398	-3.72302009	-5.73280131	-5.29611615
16	-2.50608259	-3.45924917	-3.13015923	-3.75216355	-5.77613559	-5.32899845
17	-2.00577883	-2.70937165	-2.24679828	-2.98540673	-5.30751518	-4.89856403

Table14 $R_1 = R_2 = \text{CH}_2\text{Ph}$

Entry	IE_DFT	SAPT2+3	Exchange	Electrostatic	Induction	Dispersion
1	-1.32638541	-1.73744393	3.57047117	-1.26977485	-0.41529536	-3.62284489
2	-1.41160036	-1.88794515	3.57543398	-1.34511343	-0.41340921	-3.7048565
3	-1.48171938	-2.04899137	3.65969774	-1.44247067	-0.42409342	-3.84212501
4	-1.5758587	-2.22905016	3.71923349	-1.54002046	-0.43147845	-3.97678475
5	-1.68233203	-2.42594856	3.80344552	-1.65003128	-0.44220307	-4.13715974
6	-1.80070243	-2.64080393	3.92512797	-1.77776137	-0.45738402	-4.33078651
7	-1.92505643	-2.8734994	4.10312067	-1.92994143	-0.4785891	-4.56808954
8	-2.0731202	-3.12153459	4.34293842	-2.11183398	-0.50429965	-4.84833938
9	-2.20743374	-3.37225108	4.76311409	-2.34816692	-0.55189591	-5.23530234
10	-2.38326725	-3.58970023	5.16472507	-2.56365758	-0.58831938	-5.60244834
11	-2.55084945	-3.78521338	5.9369429	-2.87759799	-0.66100999	-6.1835483
12	-2.67695576	-3.87192702	7.108003	-3.28145462	-0.76505301	-6.93342239
13	-2.68437449	-3.73768802	8.94639423	-3.84582628	-0.92192646	-7.91632951
14	-2.50739875	-3.40070462	11.1256392	-4.53649736	-1.10419609	-8.88565034
15	-2.52066567	-3.43197324	11.1232096	-4.6178873	-1.10066684	-8.83662866
16	-2.50608259	-3.45924917	11.2068901	-4.66599706	-1.11509955	-8.8850427
17	-2.00577883	-2.70937165	14.5282713	-5.66598564	-1.38617871	-10.1854786

Table15 $R_1 = \text{CH}_2\text{CH}_2\text{Ph}$, $R_2 = \text{CH}_2\text{Ph}$

Entry	IE_DFT	SAPT2+3	SAPT2+(3)	SAPT2+	SAPT2	SAPT0
1	0.0912131	-0.14672246	0.7660778	-0.33600306	-3.64542063	-3.326751
2	-1.00835049	-1.31574289	-0.64832891	-1.57652942	-4.44922991	-4.03644136
3	-1.48693913	-1.99644007	-1.48218854	-2.29154581	-4.8664582	-4.35669541
4	-1.96399655	-2.63445822	-2.22399204	-2.94232078	-5.25521569	-4.73498222
5	-2.09035806	-2.83556315	-2.45739529	-3.14212675	-5.35369873	-4.84104838
6	-2.34218533	-3.16610003	-2.86360493	-3.4736586	-5.47586443	-4.96264397
7	-2.50923626	-3.39379849	-3.14173083	-3.69569498	-5.53699341	-5.04673786
8	-2.71953036	-3.58051212	-3.35950763	-3.87146185	-5.57270042	-5.14422763
9	-2.81784142	-3.75620803	-3.55333369	-4.03847773	-5.64475609	-5.26129302
10	-2.88381685	-3.93185352	-3.7418396	-4.20619929	-5.73189937	-5.38060149
11	-2.85352736	-4.0114729	-3.81573367	-4.27608369	-5.75191901	-5.43953932
12	-2.82556142	-4.09045058	-3.89841113	-4.34288957	-5.74118106	-5.46203168
13	-2.76843536	-4.07520763	-3.87544343	-4.31302671	-5.65664376	-5.41900463
14	-2.67436583	-3.9800944	-3.76156307	-4.20140634	-5.51383095	-5.32213715
15	-2.54790587	-3.83892797	-3.59081823	-4.0443152	-5.3580811	-5.20567414
16	-2.48219888	-3.77591497	-3.5130049	-3.96892042	-5.2566869	-5.13131466
17	-2.40602883	-3.70409765	-3.42918231	-3.88808838	-5.15978297	-5.05131541

Table16 $R_1 = \text{CH}_2\text{CH}_2\text{Ph}$, $R_2 = \text{CH}_2\text{Ph}$

Entry	IE_DFT	SAPT2+3	Exchange	Electrostatic	Induction	Dispersion
1	0.0912131	-0.14672246	25.6858343	-9.38265997	-2.3159593	-14.1339375

2	-1.00835049	-1.31574289	20.0347932	-7.26208165	-1.76440747	-12.324047
3	-1.48693913	-1.99644007	16.4126913	-5.9657043	-1.40977001	-11.0336571
4	-1.96399655	-2.63445822	13.7754373	-5.19626867	-1.20099624	-10.0126306
5	-2.09035806	-2.83556315	12.8400332	-4.91807102	-1.15579569	-9.60172958
6	-2.34218533	-3.16610003	10.8546812	-4.25219518	-1.01424213	-8.75434389
7	-2.50923626	-3.39379849	9.43662064	-3.77790311	-0.93925988	-8.11325614
8	-2.71953036	-3.58051212	8.44416533	-3.50978439	-0.89164228	-7.62325078
9	-2.81784142	-3.75620803	7.83082335	-3.43750352	-0.869603	-7.27992485
10	-2.88381685	-3.93185352	7.3931466	-3.48813764	-0.83859102	-6.99827145
11	-2.85352736	-4.0114729	7.43575908	-3.72626528	-0.84240285	-6.87856384
12	-2.82556142	-4.09045058	7.21681622	-3.87363575	-0.81199333	-6.62163772
13	-2.76843536	-4.07520763	7.27419305	-4.06841102	-0.80630822	-6.47468144
14	-2.67436583	-3.9800944	7.59488632	-4.30696749	-0.82878708	-6.43922614
15	-2.54790587	-3.83892797	8.20160769	-4.62023419	-0.87827178	-6.54202968
16	-2.48219888	-3.77591497	8.47057491	-4.81079029	-0.90175138	-6.5339482
17	-2.40602883	-3.70409765	8.71121232	-4.95248381	-0.92419507	-6.53863109

Table17 $R_1 = R_2 = \text{CH}_2\text{CH}_2\text{Ph}$

Entry	IE_DFT	SAPT2+3	SAPT2+(3)	SAPT2+	SAPT2	SAPT0
1	-2.87437764	-3.79927872	-3.46728467	-4.07574657	-6.02909238	-5.73695326
2	-2.92759653	-3.79375299	-3.47180045	-4.07596355	-6.02376592	-5.72058347
3	-2.92784355	-3.76719191	-3.45386059	-4.05553454	-6.006651	-5.68222636
4	-2.87445403	-3.72169147	-3.41567973	-4.01666851	-5.9799931	-5.62436455
5	-2.84884396	-3.68772848	-3.39100437	-3.98336035	-5.92216059	-5.54435674
6	-2.79106368	-3.66709607	-3.38750715	-3.96473705	-5.86720567	-5.45903228
7	-2.74838461	-3.66051509	-3.40256502	-3.95690512	-5.79273949	-5.35985982
8	-2.72870768	-3.68916192	-3.4563627	-3.98247217	-5.73008474	-5.27617806
9	-2.65527958	-3.72480708	-3.51429751	-4.01539677	-5.68916175	-5.20516451
10	-2.63912657	-3.76504432	-3.56187396	-4.05568736	-5.70846258	-5.21237909
11	-2.61176528	-3.82351858	-3.63215101	-4.11228855	-5.72216562	-5.21071834
12	-2.65957408	-3.86907229	-3.67243488	-4.15905438	-5.79142886	-5.29698636
13	-2.6180072	-3.96722727	-3.79138299	-4.24960119	-5.78465542	-5.26579515
14	-2.6315932	-4.04140715	-3.87414027	-4.32036964	-5.81363041	-5.29435809
15	-2.66804185	-4.06718937	-3.89845903	-4.3444641	-5.83913658	-5.34128174
16	-2.76717776	-4.10772796	-3.93783852	-4.37926306	-5.85372461	-5.39805721
17	-2.8238084	-4.11485548	-3.93678134	-4.38282701	-5.8647879	-5.44952062

Table18 $R_1 = R_2 = \text{CH}_2\text{CH}_2\text{Ph}$

Entry	IE_DFT	SAPT2+3	Exchange	Electrostatic	Induction	Dispersion
1	-2.87437764	-3.79927872	11.0702374	-4.98349698	-1.17303369	-8.71298541
2	-2.92759653	-3.79375299	10.8800627	-4.82251774	-1.15366937	-8.69762862
3	-2.92784355	-3.76719191	10.7395604	-4.67804549	-1.13601647	-8.69269039
4	-2.87445403	-3.72169147	10.646787	-4.55100188	-1.11907936	-8.69839721
5	-2.84884396	-3.68772848	10.4153146	-4.41591852	-1.08911088	-8.59801365
6	-2.79106368	-3.66709607	10.0277436	-4.22411911	-1.04745788	-8.42326263
7	-2.74838461	-3.66051509	9.46587119	-3.99601796	-0.98574569	-8.14462263
8	-2.72870768	-3.68916192	8.77342864	-3.76190616	-0.90774916	-7.79293524

9	-2.65527958	-3.72480708	8.16668888	-3.58470908	-0.84234271	-7.46444416
10	-2.63912657	-3.76504432	7.96894435	-3.54639106	-0.82006238	-7.36753524
11	-2.61176528	-3.82351858	7.62651544	-3.48586918	-0.78376597	-7.18039888
12	-2.65957408	-3.86907229	7.74513648	-3.55026893	-0.80398464	-7.2599552
13	-2.6180072	-3.96722727	7.11226465	-3.46061491	-0.73902694	-6.87985007
14	-2.6315932	-4.04140715	6.83401119	-3.43558513	-0.71899193	-6.72084128
15	-2.66804185	-4.06718937	6.83453381	-3.45108305	-0.73538635	-6.71525378
16	-2.76717776	-4.10772796	6.77996009	-3.47157813	-0.74880654	-6.66730338
17	-2.8238084	-4.11485548	6.94774834	-3.55774099	-0.78605684	-6.718806

Table19 $R_1 = R_2 = \text{CH}_2\text{Oph}$

Entry	IE_DFT	SAPT2+3	SAPT2+(3)	SAPT2+	SAPT2	SAPT0
1	-2.30475822	-3.76315024	-3.4690183	-3.9748786	-5.4617276	-5.20141695
2	-2.4501568	-3.85114752	-3.56003821	-4.07398067	-5.61176542	-5.34357928
3	-2.57859173	-3.89501922	-3.60461089	-4.1285715	-5.72607672	-5.45268301
4	-2.68345977	-3.89760443	-3.60539053	-4.1414551	-5.80435146	-5.52677365
5	-2.75007509	-3.86401765	-3.56644562	-4.11804968	-5.8552255	-5.5710777
6	-2.75871963	-3.79078979	-3.48245124	-4.0554776	-5.8856141	-5.58819179
7	-2.83265137	-3.78076263	-3.47748838	-4.05337765	-5.90869276	-5.6030915
8	-2.84609108	-3.73044341	-3.42650293	-4.0105231	-5.90515278	-5.58705155
9	-2.83591503	-3.66344557	-3.35449016	-3.94908079	-5.88362707	-5.55591682
10	-2.80011318	-3.59611015	-3.27696823	-3.88584073	-5.86549476	-5.52905817
11	-2.74234911	-3.55152865	-3.21667652	-3.84400487	-5.87581396	-5.53063844
12	-2.7169525	-3.51852345	-3.17471182	-3.81192775	-5.87067611	-5.5184089
13	-2.63997567	-3.43636216	-3.06933749	-3.72679712	-5.83842102	-5.48791478
14	-2.57900868	-3.32813367	-2.93718536	-3.6122595	-5.76533349	-5.42737727
15	-2.54905168	-3.2435674	-2.83732086	-3.52313738	-5.698353	-5.37208271
16	-2.41338566	-3.01358542	-2.56851684	-3.28113915	-5.51909807	-5.22081785
17	-2.49674377	-3.14376055	-2.72686131	-3.42066449	-5.61765862	-5.29209998

Table20 $R_1 = R_2 = \text{CH}_2\text{Oph}$

Entry	IE_DFT	SAPT2+3	Exchange	Electrostatic	Induction	Dispersion
1	-2.30475822	-3.76315024	9.68666247	-5.37996637	-0.99977954	-7.0700668
2	-2.4501568	-3.85114752	9.66734325	-5.27765828	-1.00208656	-7.23874592
3	-2.57859173	-3.89501922	9.70613943	-5.14818997	-1.01637553	-7.43659315
4	-2.68345977	-3.89760443	9.80998502	-5.00893039	-1.03986906	-7.65879
5	-2.75007509	-3.86401765	10.0111838	-4.888721	-1.07292643	-7.91355399
6	-2.75871963	-3.79078979	10.367074	-4.81628861	-1.11956331	-8.2220119
7	-2.83265137	-3.78076263	10.3031264	-4.66216905	-1.11209921	-8.30962072
8	-2.84609108	-3.73044341	10.3908592	-4.56849176	-1.11421335	-8.43859753
9	-2.83591503	-3.66344557	10.5764323	-4.5380301	-1.11958094	-8.58226685
10	-2.80011318	-3.59611015	10.880407	-4.58683754	-1.13492842	-8.75475117
11	-2.74234911	-3.55152865	11.3031334	-4.73115148	-1.16470284	-8.95880772
12	-2.7169525	-3.51852345	11.5467715	-4.80884041	-1.18030986	-9.07614462
13	-2.63997567	-3.43636216	12.1011467	-5.00932661	-1.23565017	-9.29253204
14	-2.57900868	-3.32813367	12.644086	-5.1906063	-1.29333789	-9.48827551
15	-2.54905168	-3.2435674	12.9928087	-5.29208468	-1.32964997	-9.61464148

16	-2.41338566	-3.01358542	13.8793174	-5.56748722	-1.41602361	-9.90939199
17	-2.49674377	-3.14376055	13.2462339	-5.32996152	-1.35433035	-9.70570259

The interaction energy calculated using B2PLYP functional. All the energies are in kcal/mol.

Table21 $R_1 = R_2 = \text{Ph}$

Entry	IE_DFT	SAPT2+3	SAPT2+(3)	SAPT2+	SAPT2	SAPT0
1	-3.15083682	-4.02221849	-3.79542811	-4.32600346	-6.11558978	-5.66869057
2	-3.1344325	-4.11616631	-3.91784175	-4.40558973	-6.05496659	-5.62551819
3	-3.01114498	-4.09076178	-3.90428953	-4.36436361	-5.90713735	-5.48975544
4	-2.82349911	-3.99529738	-3.80968571	-4.2538805	-5.71610015	-5.30608582
5	-2.60088344	-3.85631253	-3.66405607	-4.1014647	-5.50326934	-5.09753096
6	-2.46527666	-3.82918438	-3.64841792	-4.06174452	-5.3543318	-4.95711402
7	-2.33481885	-3.79263617	-3.62114381	-4.01525757	-5.21282806	-4.8231893
8	-2.21365489	-3.72981286	-3.56436528	-3.94327473	-5.0602222	-4.68152181
9	-2.11091055	-3.6489887	-3.48805958	-3.85384902	-4.89958899	-4.53573441
10	-2.0289766	-3.54514758	-3.38676096	-3.74112806	-4.72522834	-4.38162795
11	-1.96952865	-3.43051188	-3.27405612	-3.61815017	-4.54675399	-4.22702772
12	-1.62992777	-2.82948242	-2.60851325	-3.00763282	-4.02050764	-3.73844389
13	-1.13735712	-2.10782973	-1.79252685	-2.26737011	-3.39525272	-3.15539202
14	-0.47341132	-1.31272917	-0.88715688	-1.44704373	-2.67149654	-2.46517657
15	0.40997959	-0.42122167	0.11512846	-0.52754148	-1.77240862	-1.6046412
16	2.05336796	1.09200212	1.80126597	1.03978795	-0.2151072	-0.09217162
17	2.13589214	1.32903382	2.04007777	1.27879889	0.08451243	0.15179745

Table22 $R_1 = R_2 = \text{Ph}$

Entry	IE_DFT	SAPT2+3	Exchange	Electrostatic	Induction	Dispersion
1	-3.15083682	-4.02221849	8.65799143	-3.87255753	-0.92002108	-7.88763132
2	-3.1344325	-4.11616631	7.74113824	-3.66885215	-0.85017567	-7.33827673
3	-3.01114498	-4.09076178	7.25195355	-3.60393369	-0.80981927	-6.92896237
4	-2.82349911	-3.99529738	7.06602499	-3.63799819	-0.79135469	-6.6319695
5	-2.60088344	-3.85631253	7.09749587	-3.73698893	-0.79002746	-6.42679202
6	-2.46527666	-3.82918438	6.68429522	-3.73456313	-0.74453574	-6.03438072
7	-2.33481885	-3.79263617	6.3571176	-3.73874574	-0.70913697	-5.70187105
8	-2.21365489	-3.72981286	6.12665238	-3.74280219	-0.6844007	-5.42926235
9	-2.11091055	-3.6489887	5.9446834	-3.72843976	-0.66647902	-5.19875331
10	-2.0289766	-3.54514758	5.81604668	-3.69546094	-0.65586184	-5.00987148
11	-1.96952865	-3.43051188	5.70896088	-3.63565229	-0.65010772	-4.85371276
12	-1.62992777	-2.82948242	7.3306591	-3.96595764	-0.78504363	-5.40914024
13	-1.13735712	-2.10782973	9.59853435	-4.55365943	-0.97557663	-6.17712803
14	-0.47341132	-1.31272917	12.1777297	-5.27473965	-1.17868223	-7.03703696
15	0.40997959	-0.42122167	14.8736412	-6.02313086	-1.3968657	-7.87486629
16	2.05336796	1.09200212	19.1368989	-7.17132277	-1.80289165	-9.07068235
17	2.13589214	1.32903382	19.3439033	-7.15659056	-1.81083673	-9.04744221

Table23 $R_1 = R_2 = \text{CH}_2\text{Ph}$

Entry	IE_DFT	SAPT2+3	SAPT2+(3)	SAPT2+	SAPT2	SAPT0
1	-1.33699227	-1.73744393	-1.64270878	-1.87614595	-2.35024364	-2.09515196
2	-1.42458491	-1.88794515	-1.79588997	-2.03402399	-2.55730616	-2.28464021
3	-1.50859512	-2.04899137	-1.9569141	-2.20417059	-2.78728801	-2.49108487
4	-1.61298088	-2.22905016	-2.13804096	-2.39341532	-3.03672735	-2.71866353
5	-1.7317854	-2.42594856	-2.33546808	-2.60046328	-3.30942077	-2.96874411
6	-1.86193552	-2.64080393	-2.54996845	-2.82671954	-3.60839802	-3.24442966
7	-2.00381449	-2.8734994	-2.78084226	-3.07237133	-3.93621008	-3.54858617
8	-2.16506834	-3.12153459	-3.02519921	-3.33449228	-4.28898019	-3.88027916
9	-2.32693909	-3.37225108	-3.26689279	-3.6031915	-4.67710002	-4.24065507
10	-2.50930598	-3.58970023	-3.47501624	-3.83612479	-5.01795711	-4.56707603
11	-2.70469446	-3.78521338	-3.64938108	-4.05211213	-5.39974264	-4.93432518
12	-2.86200613	-3.87192702	-3.69908748	-4.15828422	-5.71068588	-5.24051728
13	-2.90256417	-3.73768802	-3.49981036	-4.03746874	-5.8436076	-5.38587398
14	-2.7459192	-3.40070462	-3.07812375	-3.69868774	-5.73798836	-5.30086287
15	-2.72347427	-3.43197324	-3.10540398	-3.72302009	-5.73280131	-5.29611615
16	-2.71592965	-3.45924917	-3.13015923	-3.75216355	-5.77613559	-5.32899845
17	-2.25633121	-2.70937165	-2.24679828	-2.98540673	-5.30751518	-4.89856403

Table24 $R_1 = R_2 = \text{CH}_2\text{Ph}$

Entry	IE_DFT	SAPT2+3	Exchange	Electrostatic	Induction	Dispersion
1	-1.33699227	-1.73744393	3.57047117	-1.26977485	-0.41529536	-3.62284489
2	-1.42458491	-1.88794515	3.57543398	-1.34511343	-0.41340921	-3.7048565
3	-1.50859512	-2.04899137	3.65969774	-1.44247067	-0.42409342	-3.84212501
4	-1.61298088	-2.22905016	3.71923349	-1.54002046	-0.43147845	-3.97678475
5	-1.7317854	-2.42594856	3.80344552	-1.65003128	-0.44220307	-4.13715974
6	-1.86193552	-2.64080393	3.92512797	-1.77776137	-0.45738402	-4.33078651
7	-2.00381449	-2.8734994	4.10312067	-1.92994143	-0.4785891	-4.56808954
8	-2.16506834	-3.12153459	4.34293842	-2.11183398	-0.50429965	-4.84833938
9	-2.32693909	-3.37225108	4.76311409	-2.34816692	-0.55189591	-5.23530234
10	-2.50930598	-3.58970023	5.16472507	-2.56365758	-0.58831938	-5.60244834
11	-2.70469446	-3.78521338	5.9369429	-2.87759799	-0.66100999	-6.1835483
12	-2.86200613	-3.87192702	7.108003	-3.28145462	-0.76505301	-6.93342239
13	-2.90256417	-3.73768802	8.94639423	-3.84582628	-0.92192646	-7.91632951
14	-2.7459192	-3.40070462	11.1256392	-4.53649736	-1.10419609	-8.88565034
15	-2.72347427	-3.43197324	11.1232096	-4.6178873	-1.10066684	-8.83662866
16	-2.71592965	-3.45924917	11.2068901	-4.66599706	-1.11509955	-8.8850427
17	-2.25633121	-2.70937165	14.5282713	-5.66598564	-1.38617871	-10.1854786

Table25 $R_1 = \text{CH}_2\text{CH}_2\text{Ph}$, $R_2 = \text{CH}_2\text{Ph}$

Entry	IE_DFT	SAPT2+3	SAPT2+(3)	SAPT2+	SAPT2	SAPT0
1	-0.33406345	-0.14672246	0.7660778	-0.33600306	-3.64542063	-3.326751
2	-1.33053337	-1.31574289	-0.64832891	-1.57652942	-4.44922991	-4.03644136
3	-1.77423346	-1.99644007	-1.48218854	-2.29154581	-4.8664582	-4.35669541
4	-2.18981333	-2.63445822	-2.22399204	-2.94232078	-5.25521569	-4.73498222
5	-2.31390886	-2.83556315	-2.45739529	-3.14212675	-5.35369873	-4.84104838
6	-2.5441273	-3.16610003	-2.86360493	-3.4736586	-5.47586443	-4.96264397

7	-2.71304544	-3.39379849	-3.14173083	-3.69569498	-5.53699341	-5.04673786
8	-2.89417174	-3.58051212	-3.35950763	-3.87146185	-5.57270042	-5.14422763
9	-2.99191957	-3.75620803	-3.55333369	-4.03847773	-5.64475609	-5.26129302
10	-3.04439712	-3.93185352	-3.7418396	-4.20619929	-5.73189937	-5.38060149
11	-3.01012134	-4.0114729	-3.81573367	-4.27608369	-5.75191901	-5.43953932
12	-2.96876236	-4.09045058	-3.89841113	-4.34288957	-5.74118106	-5.46203168
13	-2.90348642	-4.07520763	-3.87544343	-4.31302671	-5.65664376	-5.41900463
14	-2.8099806	-3.9800944	-3.76156307	-4.20140634	-5.51383095	-5.32213715
15	-2.6862441	-3.83892797	-3.59081823	-4.0443152	-5.3580811	-5.20567414
16	-2.6109887	-3.77591497	-3.5130049	-3.96892042	-5.2566869	-5.13131466
17	-2.5273886	-3.70409765	-3.42918231	-3.88808838	-5.15978297	-5.05131541

Table26 $R_1 = \text{CH}_2\text{CH}_2\text{Ph}$, $R_2 = \text{CH}_2\text{Ph}$

Entry	IE_DFT	SAPT2+3	Exchange	Electrostatic	Induction	Dispersion
1	-0.33406345	-0.14672246	25.6858343	-9.38265997	-2.3159593	-14.1339375
2	-1.33053337	-1.31574289	20.0347932	-7.26208165	-1.76440747	-12.324047
3	-1.77423346	-1.99644007	16.4126913	-5.9657043	-1.40977001	-11.0336571
4	-2.18981333	-2.63445822	13.7754373	-5.19626867	-1.20099624	-10.0126306
5	-2.31390886	-2.83556315	12.8400332	-4.91807102	-1.15579569	-9.60172958
6	-2.5441273	-3.16610003	10.8546812	-4.25219518	-1.01424213	-8.75434389
7	-2.71304544	-3.39379849	9.43662064	-3.77790311	-0.93925988	-8.11325614
8	-2.89417174	-3.58051212	8.44416533	-3.50978439	-0.89164228	-7.62325078
9	-2.99191957	-3.75620803	7.83082335	-3.43750352	-0.869603	-7.27992485
10	-3.04439712	-3.93185352	7.3931466	-3.48813764	-0.83859102	-6.99827145
11	-3.01012134	-4.0114729	7.43575908	-3.72626528	-0.84240285	-6.87856384
12	-2.96876236	-4.09045058	7.21681622	-3.87363575	-0.81199333	-6.62163772
13	-2.90348642	-4.07520763	7.27419305	-4.06841102	-0.80630822	-6.47468144
14	-2.8099806	-3.9800944	7.59488632	-4.30696749	-0.82878708	-6.43922614
15	-2.6862441	-3.83892797	8.20160769	-4.62023419	-0.87827178	-6.54202968
16	-2.6109887	-3.77591497	8.47057491	-4.81079029	-0.90175138	-6.5339482
17	-2.5273886	-3.70409765	8.71121232	-4.95248381	-0.92419507	-6.53863109

Table27 $R_1 = R_2 = \text{CH}_2\text{CH}_2\text{Ph}$

Entry	IE_DFT	SAPT2+3	SAPT2+(3)	SAPT2+	SAPT2	SAPT0
1	-3.04775282	-3.79927872	-3.46728467	-4.07574657	-6.02909238	-5.73695326
2	-3.08940689	-3.79375299	-3.47180045	-4.07596355	-6.02376592	-5.72058347
3	-3.09490092	-3.76719191	-3.45386059	-4.05553454	-6.006651	-5.68222636
4	-3.06062727	-3.72169147	-3.41567973	-4.01666851	-5.9799931	-5.62436455
5	-3.02609414	-3.68772848	-3.39100437	-3.98336035	-5.92216059	-5.54435674
6	-2.97807179	-3.66709607	-3.38750715	-3.96473705	-5.86720567	-5.45903228
7	-2.92967976	-3.66051509	-3.40256502	-3.95690512	-5.79273949	-5.35985982
8	-2.8908539	-3.68916192	-3.4563627	-3.98247217	-5.73008474	-5.27617806
9	-2.8188313	-3.72480708	-3.51429751	-4.01539677	-5.68916175	-5.20516451
10	-2.80513439	-3.76504432	-3.56187396	-4.05568736	-5.70846258	-5.21237909
11	-2.77349668	-3.82351858	-3.63215101	-4.11228855	-5.72216562	-5.21071834
12	-2.83288628	-3.86907229	-3.67243488	-4.15905438	-5.79142886	-5.29698636
13	-2.76740958	-3.96722727	-3.79138299	-4.24960119	-5.78465542	-5.26579515

14	-2.7730348	-4.04140715	-3.87414027	-4.32036964	-5.81363041	-5.29435809
15	-2.82103502	-4.06718937	-3.89845903	-4.3444641	-5.83913658	-5.34128174
16	-2.91131008	-4.10772796	-3.93783852	-4.37926306	-5.85372461	-5.39805721
17	-2.97447543	-4.11485548	-3.93678134	-4.38282701	-5.8647879	-5.44952062

Table28 $R_1 = R_2 = \text{CH}_2\text{CH}_2\text{Ph}$

Entry	IE_DFT	SAPT2+3	Exchange	Electrostatic	Induction	Dispersion
1	-3.04775282	-3.79927872	11.0702374	-4.98349698	-1.17303369	-8.71298541
2	-3.08940689	-3.79375299	10.8800627	-4.82251774	-1.15366937	-8.69762862
3	-3.09490092	-3.76719191	10.7395604	-4.67804549	-1.13601647	-8.69269039
4	-3.06062727	-3.72169147	10.646787	-4.55100188	-1.11907936	-8.69839721
5	-3.02609414	-3.68772848	10.4153146	-4.41591852	-1.08911088	-8.59801365
6	-2.97807179	-3.66709607	10.0277436	-4.22411911	-1.04745788	-8.42326263
7	-2.92967976	-3.66051509	9.46587119	-3.99601796	-0.98574569	-8.14462263
8	-2.8908539	-3.68916192	8.77342864	-3.76190616	-0.90774916	-7.79293524
9	-2.8188313	-3.72480708	8.16668888	-3.58470908	-0.84234271	-7.46444416
10	-2.80513439	-3.76504432	7.96894435	-3.54639106	-0.82006238	-7.36753524
11	-2.77349668	-3.82351858	7.62651544	-3.48586918	-0.78376597	-7.18039888
12	-2.83288628	-3.86907229	7.74513648	-3.55026893	-0.80398464	-7.2599552
13	-2.76740958	-3.96722727	7.11226465	-3.46061491	-0.73902694	-6.87985007
14	-2.7730348	-4.04140715	6.83401119	-3.43558513	-0.71899193	-6.72084128
15	-2.82103502	-4.06718937	6.83453381	-3.45108305	-0.73538635	-6.71525378
16	-2.91131008	-4.10772796	6.77996009	-3.47157813	-0.74880654	-6.66730338
17	-2.97447543	-4.11485548	6.94774834	-3.55774099	-0.78605684	-6.718806

Table29 $R_1 = R_2 = \text{CH}_2\text{Oph}$

Entry	IE_DFT	SAPT2+3	SAPT2+(3)	SAPT2+	SAPT2	SAPT0
1	-2.42181881	-3.76315024	-3.4690183	-3.9748786	-5.4617276	-5.20141695
2	-2.56346289	-3.85114752	-3.56003821	-4.07398067	-5.61176542	-5.34357928
3	-2.69722332	-3.89501922	-3.60461089	-4.1285715	-5.72607672	-5.45268301
4	-2.81186493	-3.89760443	-3.60539053	-4.1414551	-5.80435146	-5.52677365
5	-2.89636791	-3.86401765	-3.56644562	-4.11804968	-5.8552255	-5.5710777
6	-2.93699149	-3.79078979	-3.48245124	-4.0554776	-5.8856141	-5.58819179
7	-3.00612728	-3.78076263	-3.47748838	-4.05337765	-5.90869276	-5.6030915
8	-3.02705426	-3.73044341	-3.42650293	-4.0105231	-5.90515278	-5.58705155
9	-3.02157275	-3.66344557	-3.35449016	-3.94908079	-5.88362707	-5.55591682
10	-2.98860722	-3.59611015	-3.27696823	-3.88584073	-5.86549476	-5.52905817
11	-2.93658064	-3.55152865	-3.21667652	-3.84400487	-5.87581396	-5.53063844
12	-2.90687371	-3.51852345	-3.17471182	-3.81192775	-5.87067611	-5.5184089
13	-2.83702865	-3.43636216	-3.06933749	-3.72679712	-5.83842102	-5.48791478
14	-2.77708734	-3.32813367	-2.93718536	-3.6122595	-5.76533349	-5.42737727
15	-2.74414239	-3.2435674	-2.83732086	-3.52313738	-5.698353	-5.37208271
16	-2.61979347	-3.01358542	-2.56851684	-3.28113915	-5.51909807	-5.22081785
17	-2.69605494	-3.14376055	-2.72686131	-3.42066449	-5.61765862	-5.29209998

Table30 $R_1 = R_2 = \text{CH}_2\text{Oph}$

Entry	IE_DFT	SAPT2+3	Exchange	Electrostatic	Induction	Dispersion
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1	-2.42181881	-3.76315024	9.68666247	-5.37996637	-0.99977954	-7.0700668
2	-2.56346289	-3.85114752	9.66734325	-5.27765828	-1.00208656	-7.23874592
3	-2.69722332	-3.89501922	9.70613943	-5.14818997	-1.01637553	-7.43659315
4	-2.81186493	-3.89760443	9.80998502	-5.00893039	-1.03986906	-7.65879
5	-2.89636791	-3.86401765	10.0111838	-4.888721	-1.07292643	-7.91355399
6	-2.93699149	-3.79078979	10.367074	-4.81628861	-1.11956331	-8.2220119
7	-3.00612728	-3.78076263	10.3031264	-4.66216905	-1.11209921	-8.30962072
8	-3.02705426	-3.73044341	10.3908592	-4.56849176	-1.11421335	-8.43859753
9	-3.02157275	-3.66344557	10.5764323	-4.5380301	-1.11958094	-8.58226685
10	-2.98860722	-3.59611015	10.880407	-4.58683754	-1.13492842	-8.75475117
11	-2.93658064	-3.55152865	11.3031334	-4.73115148	-1.16470284	-8.95880772
12	-2.90687371	-3.51852345	11.5467715	-4.80884041	-1.18030986	-9.07614462
13	-2.83702865	-3.43636216	12.1011467	-5.00932661	-1.23565017	-9.29253204
14	-2.77708734	-3.32813367	12.644086	-5.1906063	-1.29333789	-9.48827551
15	-2.74414239	-3.2435674	12.9928087	-5.29208468	-1.32964997	-9.61464148
16	-2.61979347	-3.01358542	13.8793174	-5.56748722	-1.41602361	-9.90939199
17	-2.69605494	-3.14376055	13.2462339	-5.32996152	-1.35433035	-9.70570259

The interaction energy calculated using SCS-MP2 functional. All the energies are in kcal/mol.

Table31 $R_1 = R_2 = \text{Ph}$

Entry	IE_DFT	SAPT2+3	SAPT2+(3)	SAPT2+	SAPT2	SAPT0
1	-3.41563056	-4.02221849	-3.79542811	-4.32600346	-6.11558978	-5.66869057
2	-3.37425046	-4.11616631	-3.91784175	-4.40558973	-6.05496659	-5.62551819
3	-3.24255746	-4.09076178	-3.90428953	-4.36436361	-5.90713735	-5.48975544
4	-3.05508252	-3.99529738	-3.80968571	-4.2538805	-5.71610015	-5.30608582
5	-2.83601153	-3.85631253	-3.66405607	-4.1014647	-5.50326934	-5.09753096
6	-2.66673344	-3.82918438	-3.64841792	-4.06174452	-5.3543318	-4.95711402
7	-2.50033457	-3.79263617	-3.62114381	-4.01525757	-5.21282806	-4.8231893
8	-2.35675444	-3.72981286	-3.56436528	-3.94327473	-5.0602222	-4.68152181
9	-2.23737819	-3.6489887	-3.48805958	-3.85384902	-4.89958899	-4.53573441
10	-2.14168819	-3.54514758	-3.38676096	-3.74112806	-4.72522834	-4.38162795
11	-2.07256101	-3.43051188	-3.27405612	-3.61815017	-4.54675399	-4.22702772
12	-1.75026803	-2.82948242	-2.60851325	-3.00763282	-4.02050764	-3.73844389
13	-1.28440525	-2.10782973	-1.79252685	-2.26737011	-3.39525272	-3.15539202
14	-0.62081146	-1.31272917	-0.88715688	-1.44704373	-2.67149654	-2.46517657
15	0.31074041	-0.42122167	0.11512846	-0.52754148	-1.77240862	-1.6046412
16	2.00766693	1.09200212	1.80126597	1.03978795	-0.2151072	-0.09217162
17	2.10634008	1.32903382	2.04007777	1.27879889	0.08451243	0.15179745

Table32 $R_1 = R_2 = \text{Ph}$

Entry	IE_DFT	SAPT2+3	Exchange	Electrostatic	Induction	Dispersion
1	-3.41563056	-4.02221849	8.65799143	-3.87255753	-0.92002108	-7.88763132
2	-3.37425046	-4.11616631	7.74113824	-3.66885215	-0.85017567	-7.33827673
3	-3.24255746	-4.09076178	7.25195355	-3.60393369	-0.80981927	-6.92896237
4	-3.05508252	-3.99529738	7.06602499	-3.63799819	-0.79135469	-6.6319695
5	-2.83601153	-3.85631253	7.09749587	-3.73698893	-0.79002746	-6.42679202
6	-2.66673344	-3.82918438	6.68429522	-3.73456313	-0.74453574	-6.03438072

7	-2.50033457	-3.79263617	6.3571176	-3.73874574	-0.70913697	-5.70187105
8	-2.35675444	-3.72981286	6.12665238	-3.74280219	-0.6844007	-5.42926235
9	-2.23737819	-3.6489887	5.9446834	-3.72843976	-0.66647902	-5.19875331
10	-2.14168819	-3.54514758	5.81604668	-3.69546094	-0.65586184	-5.00987148
11	-2.07256101	-3.43051188	5.70896088	-3.63565229	-0.65010772	-4.85371276
12	-1.75026803	-2.82948242	7.3306591	-3.96595764	-0.78504363	-5.40914024
13	-1.28440525	-2.10782973	9.59853435	-4.55365943	-0.97557663	-6.17712803
14	-0.62081146	-1.31272917	12.1777297	-5.27473965	-1.17868223	-7.03703696
15	0.31074041	-0.42122167	14.8736412	-6.02313086	-1.3968657	-7.87486629
16	2.00766693	1.09200212	19.1368989	-7.17132277	-1.80289165	-9.07068235
17	2.10634008	1.32903382	19.3439033	-7.15659056	-1.81083673	-9.04744221

Table33 $R_1 = R_2 = \text{CH}_2\text{Ph}$

Entry	IE_DFT	SAPT2+3	SAPT2+(3)	SAPT2+	SAPT2	SAPT0
1	-1.26560109	-1.73744393	-1.64270878	-1.87614595	-2.35024364	-2.09515196
2	-1.36773055	-1.88794515	-1.79588997	-2.03402399	-2.55730616	-2.28464021
3	-1.48157973	-2.04899137	-1.9569141	-2.20417059	-2.78728801	-2.49108487
4	-1.61407888	-2.22905016	-2.13804096	-2.39341532	-3.03672735	-2.71866353
5	-1.76150499	-2.42594856	-2.33546808	-2.60046328	-3.30942077	-2.96874411
6	-1.91987739	-2.64080393	-2.54996845	-2.82671954	-3.60839802	-3.24442966
7	-2.09187638	-2.8734994	-2.78084226	-3.07237133	-3.93621008	-3.54858617
8	-2.28049482	-3.12153459	-3.02519921	-3.33449228	-4.28898019	-3.88027916
9	-2.4940408	-3.37225108	-3.26689279	-3.6031915	-4.67710002	-4.24065507
10	-2.69606207	-3.58970023	-3.47501624	-3.83612479	-5.01795711	-4.56707603
11	-2.93147873	-3.78521338	-3.64938108	-4.05211213	-5.39974264	-4.93432518
12	-3.14657533	-3.87192702	-3.69908748	-4.15828422	-5.71068588	-5.24051728
13	-3.24914373	-3.73768802	-3.49981036	-4.03746874	-5.8436076	-5.38587398
14	-3.13343881	-3.40070462	-3.07812375	-3.69868774	-5.73798836	-5.30086287
15	-3.06869613	-3.43197324	-3.10540398	-3.72302009	-5.73280131	-5.29611615
16	-3.0689168	-3.45924917	-3.13015923	-3.75216355	-5.77613559	-5.32899845
17	-2.67263049	-2.70937165	-2.24679828	-2.98540673	-5.30751518	-4.89856403

Table34 $R_1 = R_2 = \text{CH}_2\text{Ph}$

Entry	IE_DFT	SAPT2+3	Exchange	Electrostatic	Induction	Dispersion
1	-1.26560109	-1.73744393	3.57047117	-1.26977485	-0.41529536	-3.62284489
2	-1.36773055	-1.88794515	3.57543398	-1.34511343	-0.41340921	-3.7048565
3	-1.48157973	-2.04899137	3.65969774	-1.44247067	-0.42409342	-3.84212501
4	-1.61407888	-2.22905016	3.71923349	-1.54002046	-0.43147845	-3.97678475
5	-1.76150499	-2.42594856	3.80344552	-1.65003128	-0.44220307	-4.13715974
6	-1.91987739	-2.64080393	3.92512797	-1.77776137	-0.45738402	-4.33078651
7	-2.09187638	-2.8734994	4.10312067	-1.92994143	-0.4785891	-4.56808954
8	-2.28049482	-3.12153459	4.34293842	-2.11183398	-0.50429965	-4.84833938
9	-2.4940408	-3.37225108	4.76311409	-2.34816692	-0.55189591	-5.23530234
10	-2.69606207	-3.58970023	5.16472507	-2.56365758	-0.58831938	-5.60244834
11	-2.93147873	-3.78521338	5.9369429	-2.87759799	-0.66100999	-6.1835483
12	-3.14657533	-3.87192702	7.108003	-3.28145462	-0.76505301	-6.93342239
13	-3.24914373	-3.73768802	8.94639423	-3.84582628	-0.92192646	-7.91632951

14	-3.13343881	-3.40070462	11.1256392	-4.53649736	-1.10419609	-8.88565034
15	-3.06869613	-3.43197324	11.1232096	-4.6178873	-1.10066684	-8.83662866
16	-3.0689168	-3.45924917	11.2068901	-4.66599706	-1.11509955	-8.8850427
17	-2.67263049	-2.70937165	14.5282713	-5.66598564	-1.38617871	-10.1854786

Table35 $R_1 = \text{CH}_2\text{CH}_2\text{Ph}$, $R_2 = \text{CH}_2\text{Ph}$

Entry	IE_DFT	SAPT2+3	SAPT2+(3)	SAPT2+	SAPT2	SAPT0
1	-1.0322168	-0.14672246	0.7660778	-0.33600306	-3.64542063	-3.326751
2	-1.8927334	-1.31574289	-0.64832891	-1.57652942	-4.44922991	-4.03644136
3	-2.277883	-1.99644007	-1.48218854	-2.29154581	-4.8664582	-4.35669541
4	-2.59928838	-2.63445822	-2.22399204	-2.94232078	-5.25521569	-4.73498222
5	-2.70710068	-2.83556315	-2.45739529	-3.14212675	-5.35369873	-4.84104838
6	-2.89267442	-3.16610003	-2.86360493	-3.4736586	-5.47586443	-4.96264397
7	-3.04445495	-3.39379849	-3.14173083	-3.69569498	-5.53699341	-5.04673786
8	-3.17662521	-3.58051212	-3.35950763	-3.87146185	-5.57270042	-5.14422763
9	-3.26736551	-3.75620803	-3.55333369	-4.03847773	-5.64475609	-5.26129302
10	-3.29438713	-3.93185352	-3.7418396	-4.20619929	-5.73189937	-5.38060149
11	-3.23694594	-4.0114729	-3.81573367	-4.27608369	-5.75191901	-5.43953932
12	-3.17138912	-4.09045058	-3.89841113	-4.34288957	-5.74118106	-5.46203168
13	-3.088037	-4.07520763	-3.87544343	-4.31302671	-5.65664376	-5.41900463
14	-2.99049547	-3.9800944	-3.76156307	-4.20140634	-5.51383095	-5.32213715
15	-2.86719289	-3.83892797	-3.59081823	-4.0443152	-5.3580811	-5.20567414
16	-2.77599596	-3.77591497	-3.5130049	-3.96892042	-5.2566869	-5.13131466
17	-2.68029575	-3.70409765	-3.42918231	-3.88808838	-5.15978297	-5.05131541

Table36 $R_1 = \text{CH}_2\text{CH}_2\text{Ph}$, $R_2 = \text{CH}_2\text{Ph}$

Entry	IE_DFT	SAPT2+3	Exchange	Electrostatic	Induction	Dispersion
1	-1.0322168	-0.14672246	25.6858343	-9.38265997	-2.3159593	-14.1339375
2	-1.8927334	-1.31574289	20.0347932	-7.26208165	-1.76440747	-12.324047
3	-2.277883	-1.99644007	16.4126913	-5.9657043	-1.40977001	-11.0336571
4	-2.59928838	-2.63445822	13.7754373	-5.19626867	-1.20099624	-10.0126306
5	-2.70710068	-2.83556315	12.8400332	-4.91807102	-1.15579569	-9.60172958
6	-2.89267442	-3.16610003	10.8546812	-4.25219518	-1.01424213	-8.75434389
7	-3.04445495	-3.39379849	9.43662064	-3.77790311	-0.93925988	-8.11325614
8	-3.17662521	-3.58051212	8.44416533	-3.50978439	-0.89164228	-7.62325078
9	-3.26736551	-3.75620803	7.83082335	-3.43750352	-0.869603	-7.27992485
10	-3.29438713	-3.93185352	7.3931466	-3.48813764	-0.83859102	-6.99827145
11	-3.23694594	-4.0114729	7.43575908	-3.72626528	-0.84240285	-6.87856384
12	-3.17138912	-4.09045058	7.21681622	-3.87363575	-0.81199333	-6.62163772
13	-3.088037	-4.07520763	7.27419305	-4.06841102	-0.80630822	-6.47468144
14	-2.99049547	-3.9800944	7.59488632	-4.30696749	-0.82878708	-6.43922614
15	-2.86719289	-3.83892797	8.20160769	-4.62023419	-0.87827178	-6.54202968
16	-2.77599596	-3.77591497	8.47057491	-4.81079029	-0.90175138	-6.5339482
17	-2.68029575	-3.70409765	8.71121232	-4.95248381	-0.92419507	-6.53863109

Table37 $R_1 = R_2 = \text{CH}_2\text{CH}_2\text{Ph}$

Entry	IE_DFT	SAPT2+3	SAPT2+(3)	SAPT2+	SAPT2	SAPT0
1	-3.33784651	-3.79927872	-3.46728467	-4.07574657	-6.02909238	-5.73695326
2	-3.37251636	-3.79375299	-3.47180045	-4.07596355	-6.02376592	-5.72058347
3	-3.38573021	-3.76719191	-3.45386059	-4.05553454	-6.006651	-5.68222636
4	-3.3804823	-3.72169147	-3.41567973	-4.01666851	-5.9799931	-5.62436455
5	-3.3371702	-3.68772848	-3.39100437	-3.98336035	-5.92216059	-5.54435674
6	-3.28988937	-3.66709607	-3.38750715	-3.96473705	-5.86720567	-5.45903228
7	-3.22957192	-3.66051509	-3.40256502	-3.95690512	-5.79273949	-5.35985982
8	-3.1725911	-3.68916192	-3.4563627	-3.98247217	-5.73008474	-5.27617806
9	-3.09172965	-3.72480708	-3.51429751	-4.01539677	-5.68916175	-5.20516451
10	-3.08417544	-3.76504432	-3.56187396	-4.05568736	-5.70846258	-5.21237909
11	-3.04390643	-3.82351858	-3.63215101	-4.11228855	-5.72216562	-5.21071834
12	-3.11899695	-3.86907229	-3.67243488	-4.15905438	-5.79142886	-5.29698636
13	-3.01697673	-3.96722727	-3.79138299	-4.24960119	-5.78465542	-5.26579515
14	-3.00856331	-4.04140715	-3.87414027	-4.32036964	-5.81363041	-5.29435809
15	-3.06576253	-4.06718937	-3.89845903	-4.3444641	-5.83913658	-5.34128174
16	-3.13820581	-4.10772796	-3.93783852	-4.37926306	-5.85372461	-5.39805721
17	-3.19917255	-4.11485548	-3.93678134	-4.38282701	-5.8647879	-5.44952062

Table38 $R_1 = R_2 = \text{CH}_2\text{CH}_2\text{Ph}$

Entry	IE_DFT	SAPT2+3	Exchange	Electrostatic	Induction	Dispersion
1	-3.33784651	-3.79927872	11.0702374	-4.98349698	-1.17303369	-8.71298541
2	-3.37251636	-3.79375299	10.8800627	-4.82251774	-1.15366937	-8.69762862
3	-3.38573021	-3.76719191	10.7395604	-4.67804549	-1.13601647	-8.69269039
4	-3.3804823	-3.72169147	10.646787	-4.55100188	-1.11907936	-8.69839721
5	-3.3371702	-3.68772848	10.4153146	-4.41591852	-1.08911088	-8.59801365
6	-3.28988937	-3.66709607	10.0277436	-4.22411911	-1.04745788	-8.42326263
7	-3.22957192	-3.66051509	9.46587119	-3.99601796	-0.98574569	-8.14462263
8	-3.1725911	-3.68916192	8.77342864	-3.76190616	-0.90774916	-7.79293524
9	-3.09172965	-3.72480708	8.16668888	-3.58470908	-0.84234271	-7.46444416
10	-3.08417544	-3.76504432	7.96894435	-3.54639106	-0.82006238	-7.36753524
11	-3.04390643	-3.82351858	7.62651544	-3.48586918	-0.78376597	-7.18039888
12	-3.11899695	-3.86907229	7.74513648	-3.55026893	-0.80398464	-7.2599552
13	-3.01697673	-3.96722727	7.11226465	-3.46061491	-0.73902694	-6.87985007
14	-3.00856331	-4.04140715	6.83401119	-3.43558513	-0.71899193	-6.72084128
15	-3.06576253	-4.06718937	6.83453381	-3.45108305	-0.73538635	-6.71525378
16	-3.13820581	-4.10772796	6.77996009	-3.47157813	-0.74880654	-6.66730338
17	-3.19917255	-4.11485548	6.94774834	-3.55774099	-0.78605684	-6.718806

Table39 $R_1 = R_2 = \text{CH}_2\text{OPh}$

Entry	IE_DFT	SAPT2+3	SAPT2+(3)	SAPT2+	SAPT2	SAPT0
1	-2.57134684	-3.76315024	-3.4690183	-3.9748786	-5.4617276	-5.20141695
2	-2.71840757	-3.85114752	-3.56003821	-4.07398067	-5.61176542	-5.34357928
3	-2.86608365	-3.89501922	-3.60461089	-4.1285715	-5.72607672	-5.45268301
4	-2.99795315	-3.89760443	-3.60539053	-4.1414551	-5.80435146	-5.52677365
5	-3.11204777	-3.86401765	-3.56644562	-4.11804968	-5.8552255	-5.5710777
6	-3.20472714	-3.79078979	-3.48245124	-4.0554776	-5.8856141	-5.58819179

7	-3.27419154	-3.78076263	-3.47748838	-4.05337765	-5.90869276	-5.6030915
8	-3.30934119	-3.73044341	-3.42650293	-4.0105231	-5.90515278	-5.58705155
9	-3.3117395	-3.66344557	-3.35449016	-3.94908079	-5.88362707	-5.55591682
10	-3.29090176	-3.59611015	-3.27696823	-3.88584073	-5.86549476	-5.52905817
11	-3.25749639	-3.55152865	-3.21667652	-3.84400487	-5.87581396	-5.53063844
12	-3.23060071	-3.51852345	-3.17471182	-3.81192775	-5.87067611	-5.5184089
13	-3.17558807	-3.43636216	-3.06933749	-3.72679712	-5.83842102	-5.48791478
14	-3.11752195	-3.32813367	-2.93718536	-3.6122595	-5.76533349	-5.42737727
15	-3.08071379	-3.2435674	-2.83732086	-3.52313738	-5.698353	-5.37208271
16	-2.97008582	-3.01358542	-2.56851684	-3.28113915	-5.51909807	-5.22081785
17	-3.03869521	-3.14376055	-2.72686131	-3.42066449	-5.61765862	-5.29209998

Table40 $R_1 = R_2 = \text{CH}_2\text{Oph}$

Entry	IE_DFT	SAPT2+3	Exchange	Electrostatic	Induction	Dispersion
1	-2.57134684	-3.76315024	9.68666247	-5.37996637	-0.99977954	-7.0700668
2	-2.71840757	-3.85114752	9.66734325	-5.27765828	-1.00208656	-7.23874592
3	-2.86608365	-3.89501922	9.70613943	-5.14818997	-1.01637553	-7.43659315
4	-2.99795315	-3.89760443	9.80998502	-5.00893039	-1.03986906	-7.65879
5	-3.11204777	-3.86401765	10.0111838	-4.888721	-1.07292643	-7.91355399
6	-3.20472714	-3.79078979	10.367074	-4.81628861	-1.11956331	-8.2220119
7	-3.27419154	-3.78076263	10.3031264	-4.66216905	-1.11209921	-8.30962072
8	-3.30934119	-3.73044341	10.3908592	-4.56849176	-1.11421335	-8.43859753
9	-3.3117395	-3.66344557	10.5764323	-4.5380301	-1.11958094	-8.58226685
10	-3.29090176	-3.59611015	10.880407	-4.58683754	-1.13492842	-8.75475117
11	-3.25749639	-3.55152865	11.3031334	-4.73115148	-1.16470284	-8.95880772
12	-3.23060071	-3.51852345	11.5467715	-4.80884041	-1.18030986	-9.07614462
13	-3.17558807	-3.43636216	12.1011467	-5.00932661	-1.23565017	-9.29253204
14	-3.11752195	-3.32813367	12.644086	-5.1906063	-1.29333789	-9.48827551
15	-3.08071379	-3.2435674	12.9928087	-5.29208468	-1.32964997	-9.61464148
16	-2.97008582	-3.01358542	13.8793174	-5.56748722	-1.41602361	-9.90939199
17	-3.03869521	-3.14376055	13.2462339	-5.32996152	-1.35433035	-9.70570259

1. Geometrical Parameters

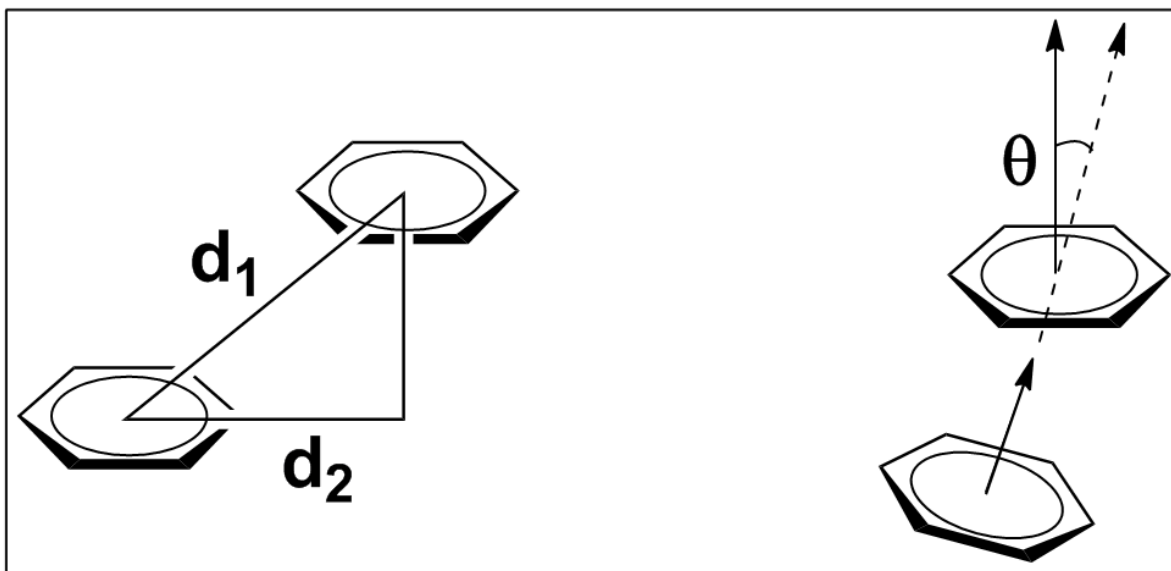


Figure 1 The direct distance (d_1) between centre of two planes, the distance between the projections of two centres in same plane is (d_2), and the angle (θ) between two planes are shown.

The direct distance (d_1) between centre of two planes, the distance between the projection of two centres in same plane (d_2), and the angle (θ) between two planes of the constrained benzene dimer and free benzene dimer are given. The distance are given in Å, and the angle is given in degree for the set of all dimers obtained from the PES.

Table41 $R_1 = R_2 = \text{Ph}$

Constrained benzene dimer along PES	Distance (d_1) Å	Distance (d_2) Å	Angle between plane (θ), degrees (°)	π - π -IE (kcal/mol)
1	3.735	2.149	1.74	-3.89446534
2	3.806	2.197	5.90	-3.80123335
3	3.878	2.245	10.07	-3.606678
4	3.949	2.293	14.23	-3.35251263
5	4.021	2.341	18.35	-3.07127909
6	4.109	2.4	21.73	-2.88622565
7	4.198	2.459	25.07	-2.71010162
8	4.286	2.518	28.43	-2.54939017
9	4.374	2.577	31.77	-2.41182568
10	4.460	2.635	35.11	-2.30019895
11	4.548	2.693	38.40	-2.20652056
12	4.540	2.685	42.73	-1.90671043
13	4.514	2.665	46.73	-1.46579673
14	4.479	2.635	48.50	-0.85586944
15	4.473	2.624	49.93	-0.03380447
16	4.466	2.613	51.11	1.48816373
17	4.536	2.653	54.82	1.59033426
Free Dimer	3.732	2.149	2.44	-3.98619542

Table42 $R_1 = R_2 = \text{CH}_2\text{Ph}$

Constrained benzene dimer along PES	Distance (d_1) Å	Distance (d_2) Å	Angle between plane (θ), degrees (°)	π - π -IE (kcal/mol)
1	4.863	3.178	64.019	-1.42563641
2	4.770	3.107	59.15	-1.53846943
3	4.676	3.036	54.17	-1.6413453
4	4.583	2.966	49.16	-1.76873225
5	4.491	2.896	44.154	-1.91268023
6	4.399	2.826	39.13	-2.07374957
7	4.306	2.757	34.11	-2.2512719
8	4.214	2.687	29.11	-2.45601406
9	4.121	2.618	24.30	-2.66139603
10	4.037	2.557	20.27	-2.91183075
11	3.935	2.483	14.846	-3.18746649
12	3.831	2.413	9.42	-3.44813228
13	3.729	2.347	5.90	-3.60570367
14	3.652	2.304	6.93	-3.55186285
15	3.658	2.32	8.23	-3.5537309
16	3.658	2.326	8.27	-3.54199105
17	3.576	2.275	9.73	-3.21680485
Free Dimer	3.732	3.178	2.44	-3.98619542

Table43 $R_1 = \text{CH}_2\text{CH}_2\text{Ph}$, $R_2 = \text{CH}_2\text{Ph}$

Constrained benzene dimer along PES	Distance (d_1) Å	Distance (d_2) Å	Angle between plane (θ), degrees (°)	π - π -IE (kcal/mol)
1	3.360	2.175	3.39	-1.75125736
2	3.414	2.123	3.40	-2.57745279
3	3.466	2.067	4.31	-2.87765985
4	3.524	2.029	5.42	-3.19674367
5	3.562	1.972	7.62	-3.26820836
6	3.627	1.901	8.75	-3.40518397
7	3.697	1.869	9.99	-3.46697149
8	3.768	1.831	11.23	-3.58165549
9	3.842	1.792	12.25	-3.6050178
10	3.909	1.778	13.17	-3.60659165
11	3.986	1.766	14.75	-3.53000773
12	4.079	1.759	15.70	-3.44490788
13	4.172	1.768	16.52	-3.34680749
14	4.257	1.779	17.10	-3.22385929
15	4.315	1.775	17.37	-3.08639226
16	4.369	1.786	18.00	-2.99999129
17	4.408	1.795	18.43	-2.91163196
Free Dimer	3.732	2.175	2.44	-3.98619542

Table44 $R_1 = R_2 = \text{CH}_2\text{CH}_2\text{Ph}$

Constrained benzene dimer along PES	Distance (d_1) Å	Distance (d_2) Å	Angle between plane (θ), degrees (°)	π - π -IE (kcal/mol)
1	3.768	1.562	3.98	-3.83836581
2	3.744	1.588	4.32	-3.89849348
3	3.724	1.619	4.545	-3.90701898
4	3.705	1.653	4.638	-3.86366824
5	3.698	1.707	6.26	-3.83499275
6	3.701	1.762	7.45	-3.76398414
7	3.716	1.822	8.77	-3.68900041
8	3.740	1.888	10.04	-3.62316997
9	3.766	1.964	10.87	-3.50653508
10	3.772	1.985	11.09	-3.47658032
11	3.789	2.021	11.68	-3.42170552
12	3.788	2.024	11.62	-3.48110389
13	3.826	2.077	12.71	-3.37438936
14	3.849	2.084	13.05	-3.35746321
15	3.864	2.118	12.64	-3.39121019
16	3.889	2.161	12.42	-3.47567213
17	3.914	2.205	12.17	-3.52676454
Free Dimer	3.732	1.562	2.44	-3.98619542

Table45 $R_1 = R_2 = \text{CH}_2\text{OPh}$

Constrained benzene dimer along PES	Distance (d_1) Å	Distance (d_2) Å	Angle between plane (θ), degrees (°)	π - π -IE (kcal/mol)
1	4.192	2.962	10.69	-2.96924022
2	4.118	2.924	10.46	-3.14776358
3	4.047	2.89	10.13	-3.31566029
4	3.978	2.86	9.72	-3.46489906
5	3.913	2.83	9.21	-3.58133671
6	3.850	2.81	8.61	-3.64545911
7	3.809	2.795	7.89	-3.73839833
8	3.774	2.784	7.16	-3.77783311
9	3.743	2.777	6.51	-3.79548085
10	3.717	2.775	5.90	-3.78890044
11	3.695	2.776	5.50	-3.76094021
12	3.677	2.778	4.94	-3.75456317
13	3.662	2.785	5.20	-3.7085385
14	3.654	2.797	5.668	-3.67553853
15	3.649	2.806	6.02	-3.66268885
16	3.643	2.818	6.91	-3.56704294
17	3.643	2.812	6.58	-3.62674654
Free Dimer	3.732	2.962	2.44	-3.98619542

2. NCI Plot

Figure 2 $R_1 = R_2 = \text{Ph}$

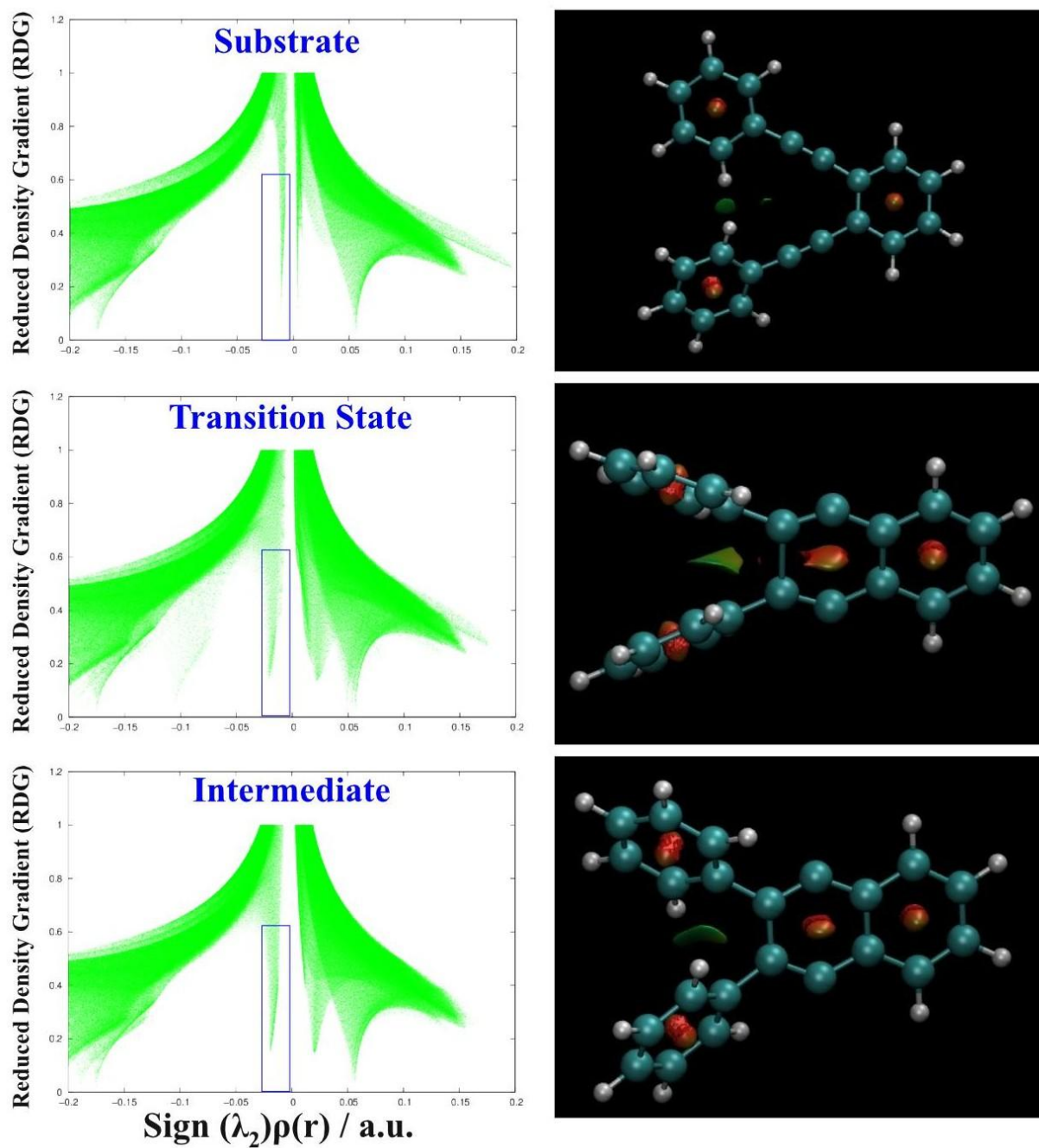


Figure 3 $R_1 = R_2 = \text{CH}_2\text{Ph}$

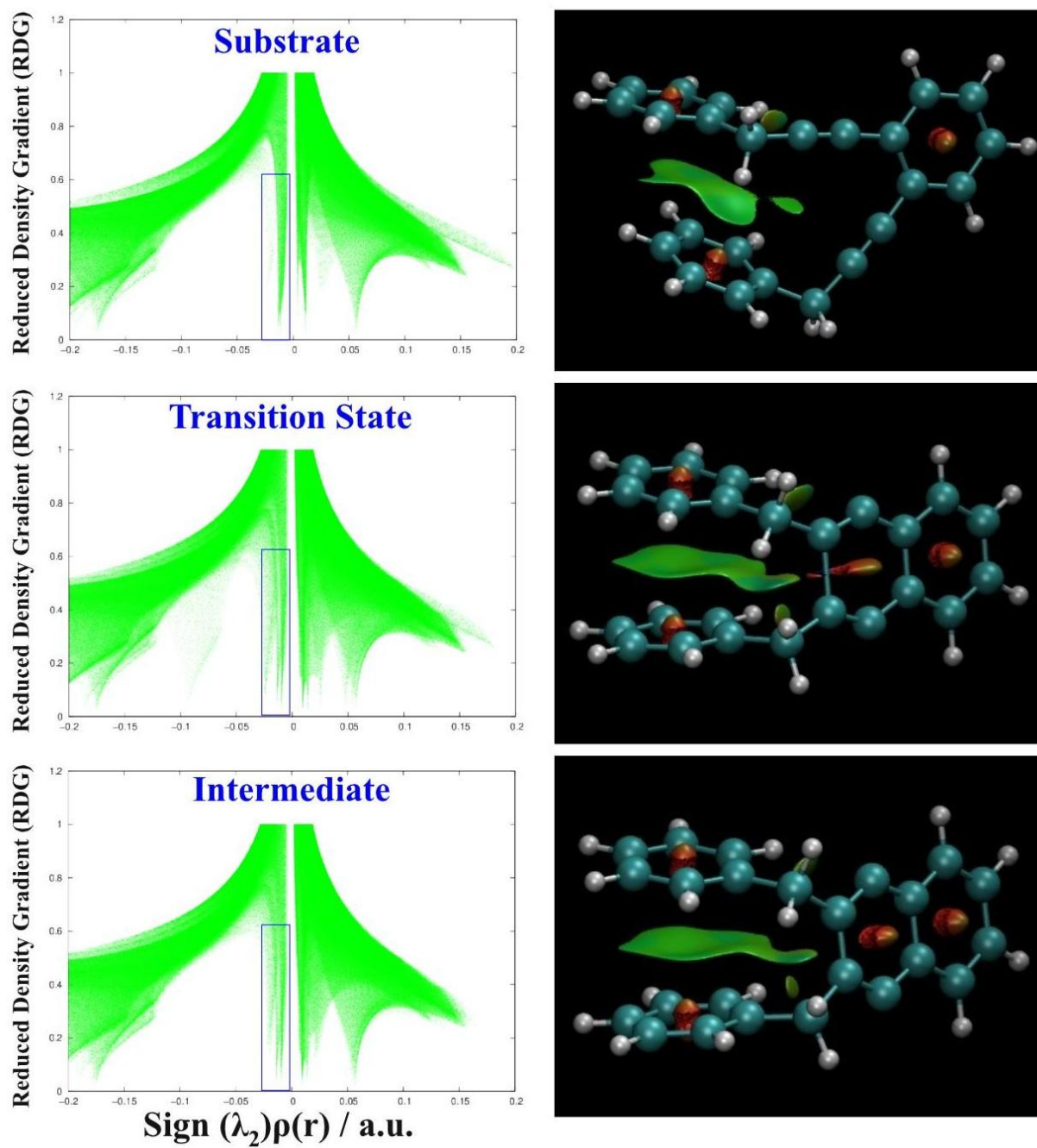


Figure 4 $R_1 = \text{CH}_2\text{CH}_2\text{Ph}$, $R_2 = \text{CH}_2\text{Ph}$

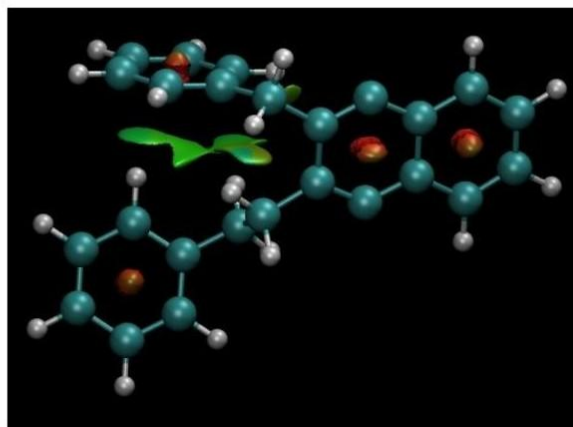
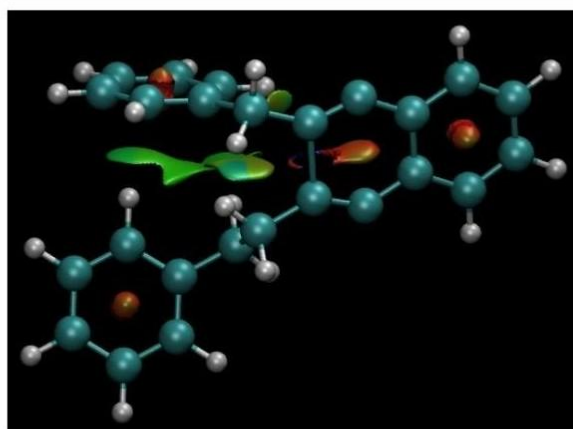
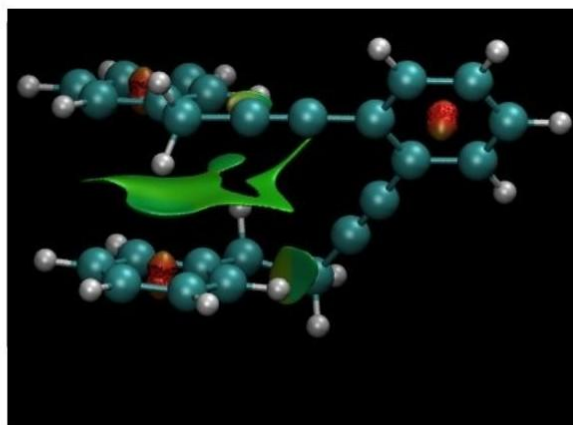
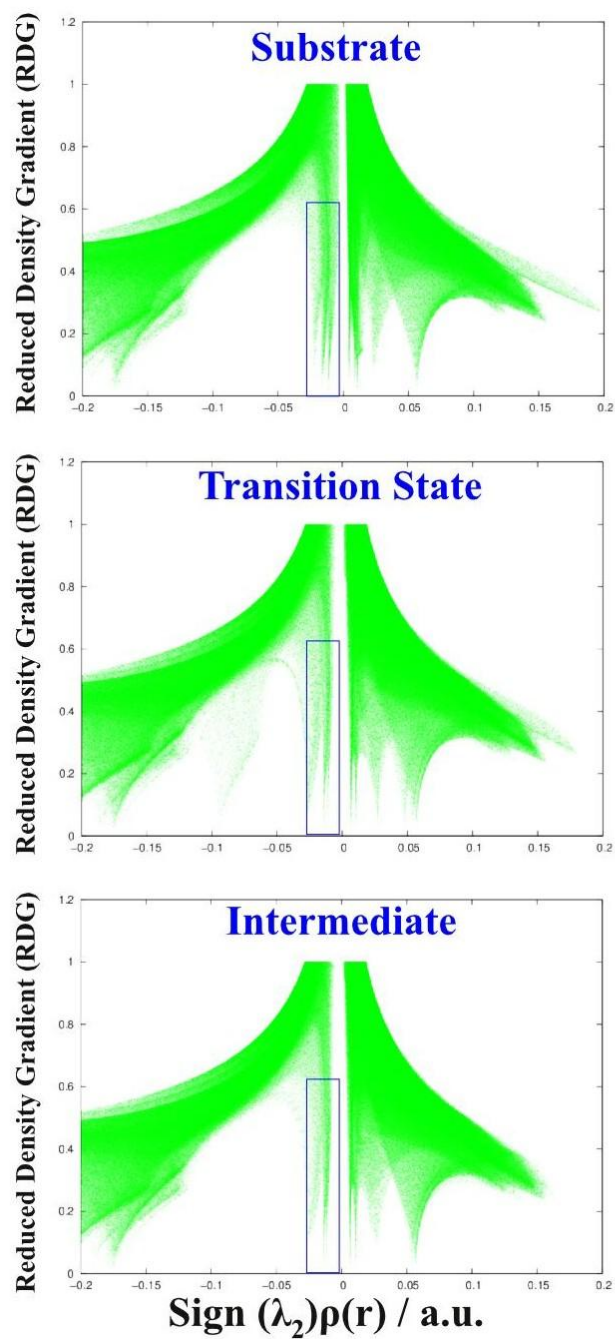


Figure 5 $R_1 = R_2 = \text{CH}_2\text{CH}_2\text{Ph}$

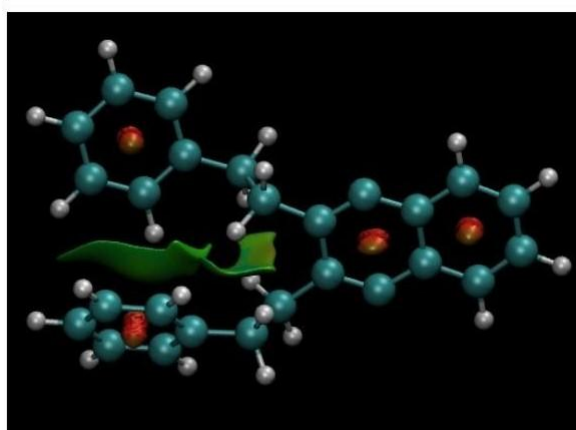
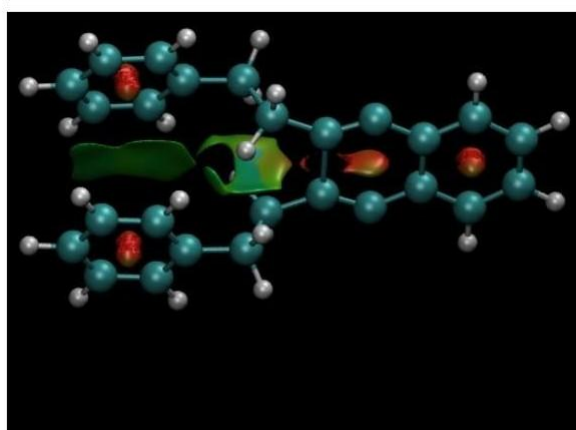
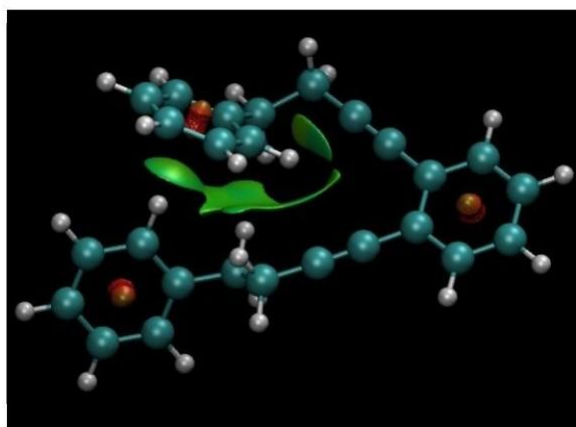
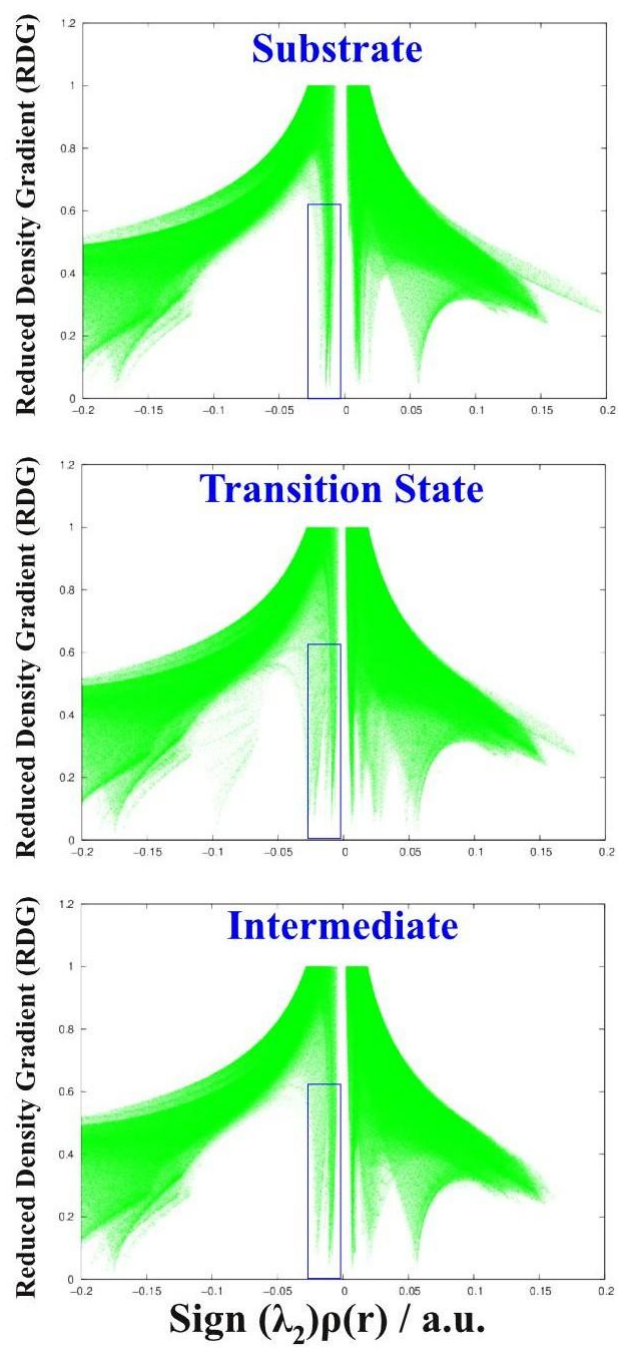
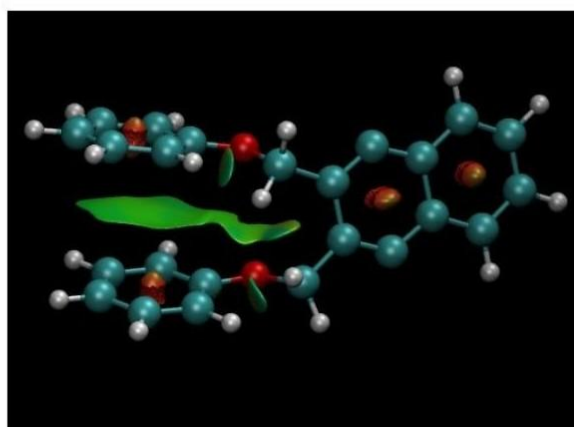
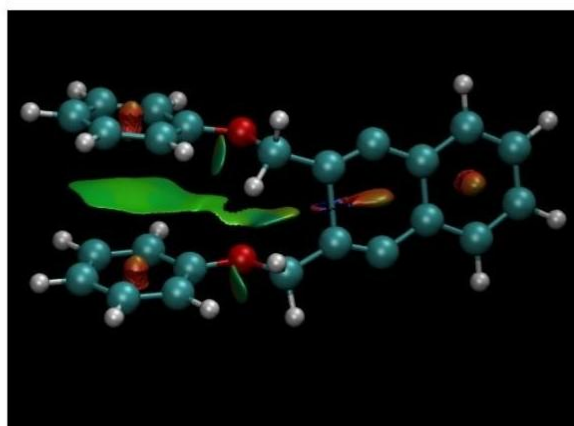
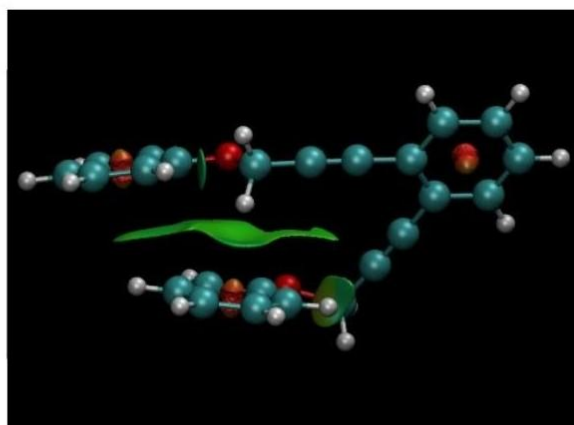
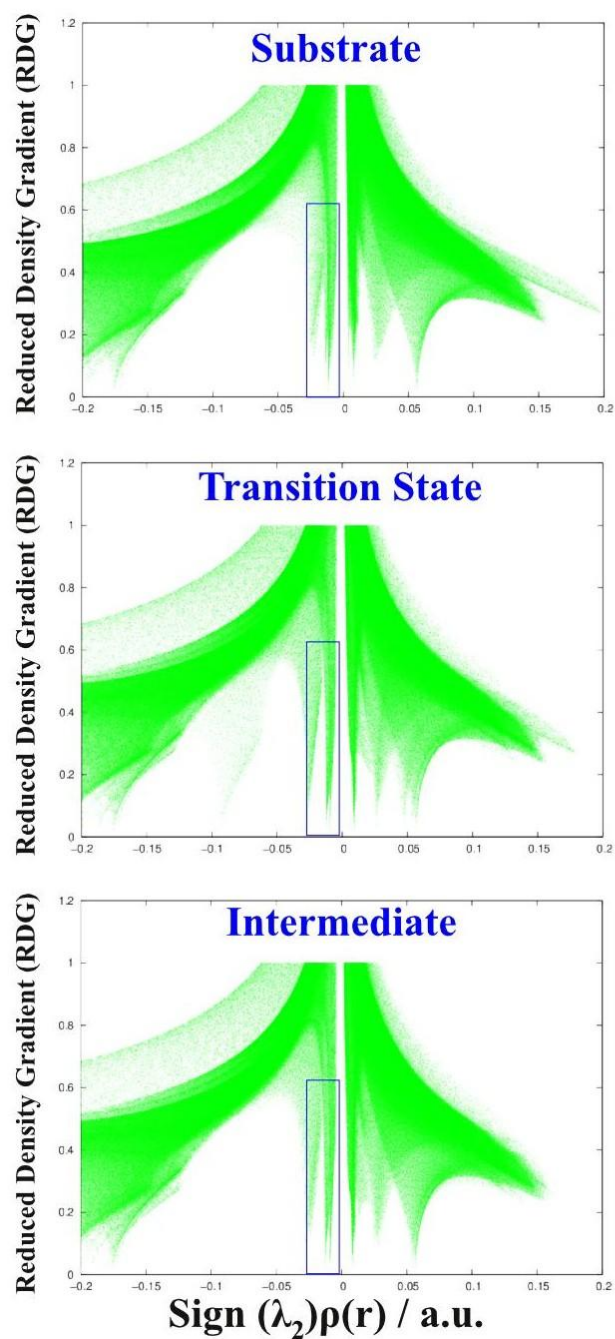


Figure 6 $R_1 = R_2 = \text{CH}_2\text{OPh}$



3. Isodesmic Reaction

Scheme 1 Isodesmic equation to study the substituent effect on π - π interaction. Here **b** is parent system.

Table 46 The stabilisation and destabilisation energy due to the substituent in substrate and transition state geometry. –ve sign implies stabilisation and +ve sign implies the destabilisation energy. Here b1, b2, b3 are the substituted geometry of the parent b. The substituted groups are F and NH₂.

Entry	Systems	$\Delta_r E_{\text{Substrate}}$	$\Delta_r E_{\text{Transition state}}$
1	b1 , R ₃ = R ₄ = F	3.88	0.92
2	b2 , R ₃ = R ₄ = NH ₂	-5.38	-0.10
3	b3 , R ₃ = F, R ₄ = NH ₂	-1.94	3.24

4. The cartesian coordinates of the optimised geometries.

R₁ = R₂ = Ph

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Substrate

C	1.14943519542930	1.65774660652516	1.26089130832616
C	0.85917578773918	1.22548994607602	-0.04752480834185
C	1.72266250662585	0.26848993960310	-0.66973972628264
C	2.84528432860823	-0.20073832737354	0.03736940079052
C	3.11350341675675	0.24604784678035	1.32843744618652
C	2.26320625019903	1.17434030501118	1.94154622440393
C	-0.24981673384975	1.72974150103214	-0.76432282697568
C	-1.16841985022847	2.14775245955125	-1.45133355984213
C	1.42598520971972	-0.18832895098406	-1.97580004700625
C	1.09921861817131	-0.55193115544704	-3.09427163791709
C	0.67021557379269	-0.93897553620919	-4.38963211609953
C	-2.21331127869439	2.59941201762757	-2.29538685621287
H	0.48679116219685	2.38548372432078	1.72807698185214
H	2.47274492060340	1.52415883168631	2.95185700907201
H	3.98708594903032	-0.13082415083960	1.85967247974944
H	3.49890633935784	-0.92641886704430	-0.44526314201308
C	-3.26520522294000	3.39808574348259	-1.79751480388213
C	-4.28110078050179	3.83112204565417	-2.64645276552662
C	-4.27034938112777	3.47836338066678	-3.99979133298861
C	-3.23098973755229	2.68860967101743	-4.50372749966418
C	-2.20901591127275	2.25253825573459	-3.66518253522978
H	-3.26930148908631	3.67051695113919	-0.74285963916727
H	-5.08762429186159	4.44879452623964	-2.25032151895080
H	-5.06752454073529	3.82006746434856	-4.65995499387940
H	-3.21498668082994	2.41236282656015	-5.55815701348082
H	-1.39241359014508	1.64478682006296	-4.05348258774525
C	1.59817785324142	-1.19778242080813	-5.42078795698176
C	1.15548210033514	-1.55239293368315	-6.69318732598506
C	-0.21277811289829	-1.65922523314656	-6.96129971163967
C	-1.14078984412532	-1.41168059653397	-5.94467797653690
C	-0.70941288909319	-1.05533884177060	-4.66934731218574
H	2.66312228916809	-1.10931997446114	-5.20780070403234
H	1.88272337395688	-1.74563180672993	-7.48199654874885
H	-0.55497905141949	-1.93690719354160	-7.95802266374734
H	-2.20878929355489	-1.49832916237125	-6.14668899132694
H	-1.42689519501543	-0.86489471217583	-3.87251324799014

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Transition state

C	1.30129037638115	1.75672537008659	1.30684527958182
C	0.94479584537511	1.30685153468555	0.02015836905740
C	1.80330308555086	0.24621068747717	-0.60538677010130
C	2.88921055216915	-0.24040910630792	0.14855154004724

C	3.18301531171037	0.24020702025183	1.41679584156660
C	2.39131350612016	1.24172351852956	1.99438821378086
C	-0.11641331823920	1.77011313380929	-0.74528520991678
C	-0.52282512846606	1.51028426622621	-1.94127251339928
C	1.42993491363971	-0.17821558542970	-1.87310290618158
C	0.44592469033514	0.12117238562430	-2.65105363639255
C	-0.10900547215661	-0.35907258251473	-3.91354522541526
C	-1.51476224650856	2.03226504159722	-2.87668916001195
H	0.69147104996752	2.53967857120814	1.75388002052892
H	2.62819685263748	1.62123011951849	2.98772945046007
H	4.03565340357335	-0.16540861734871	1.96076389188495
H	3.50070826628092	-1.02303419291575	-0.29661325320878
C	-2.86636628411559	2.09519862867645	-2.49538678677635
C	-3.82552752233448	2.57733087509958	-3.38477273424094
C	-3.45176427212728	3.00304678515718	-4.66285384097712
C	-2.10689861650738	2.95894285228657	-5.04116909717686
C	-1.14457251513258	2.47747334094856	-4.15661546986546
H	-3.15033728511604	1.75416810625002	-1.50079518621614
H	-4.87121200647963	2.61762889203071	-3.07856593031969
H	-4.20496250856183	3.37172126862099	-5.35901737827979
H	-1.80464810960702	3.29719864825841	-6.03190690610446
H	-0.09844394151384	2.43408492771619	-4.45392961504946
C	0.70601796554692	-0.40965867307663	-5.05798442652686
C	0.18528299732910	-0.85460764881325	-6.27242198971801
C	-1.15096792463539	-1.25503006309413	-6.36200585077533
C	-1.96152339319216	-1.22245874766470	-5.22370883107744
C	-1.44668403268756	-0.77742379977885	-4.00829966978610
H	1.74404043125289	-0.08873818838916	-4.98106286419279
H	0.82573471321428	-0.88573625069213	-7.15432478143557
H	-1.55726712414802	-1.59549433381461	-7.31429004042681
H	-3.00174796550102	-1.54167251078515	-5.28282904542421
H	-2.08020729405387	-0.74088267343361	-3.12377648791100

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Intermediate

C	1.22508588576948	1.74876115345274	1.21082632200490
C	0.88293012931966	1.28680573087775	-0.08513776666362
C	1.73357757619328	0.25373624574009	-0.70665715761751
C	2.83814832297487	-0.24057454392117	0.03167673202119
C	3.12347263981481	0.23900956213049	1.29424141294350
C	2.31791994830354	1.23964691753336	1.88326785208987
C	-0.18471713660331	1.72807781749674	-0.85760413670395
C	-0.52296393213826	1.35273187291639	-2.11672459902705
C	1.35057224197571	-0.15195000167492	-1.97956431950756
C	0.28331905469983	0.26138886833055	-2.70860287968209
C	-0.08149201616781	-0.37360790878773	-3.99647955877486
C	-1.60003666460516	2.03367555758450	-2.87352760471380
H	0.60457950483082	2.52307157818396	1.66090260909913
H	2.56168411186907	1.61218996028076	2.87767879014087
H	3.97938256790946	-0.15616648358000	1.84098041633586

H	3.45544826059741	-1.01420456419567	-0.42375471189198
C	-2.82244270362848	2.32113123719479	-2.24419169187126
C	-3.83649442376121	2.98519060812841	-2.93442634741198
C	-3.64266450113144	3.37713781332234	-4.26142940560277
C	-2.42435102686621	3.10614863259487	-4.89119888462014
C	-1.41107806552249	2.43897191648963	-4.20500959305913
H	-2.96910733742315	2.00729471609477	-1.21074693388353
H	-4.78219971121195	3.19611975598486	-2.43448661052784
H	-4.43595703726272	3.89420378320726	-4.80151416186070
H	-2.26079721957376	3.41692813000975	-5.92290177411977
H	-0.46313619222599	2.23337742064145	-4.70051511602948
C	0.91841781980464	-0.66778486882636	-4.93848624453101
C	0.59591861929450	-1.28696227893950	-6.14623774155127
C	-0.72971917487124	-1.62723730700138	-6.42842584169516
C	-1.72890765722009	-1.35057135851673	-5.49072297695691
C	-1.40976279334748	-0.72785037279716	-4.28506220760851
H	1.94962902458010	-0.39412552050692	-4.71388789634508
H	1.38236071560424	-1.50278947438402	-6.86990803356607
H	-0.98340529263920	-2.10902089711483	-7.37260334711354
H	-2.76372037878328	-1.62331250740169	-5.69828105914060
H	-2.19219415855818	-0.51772819054738	-3.55744953255816

$R_1 = R_2 = \text{CH}_2\text{Ph}$

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Substrate

C	1.68355539675108	1.12531069186476	1.90553386098980
C	0.75975469883256	1.55800741745894	0.95685583707101
C	0.80265028336551	1.07536465961546	-0.36387849974339
C	1.81481051808412	0.13488861523409	-0.72649135733909
C	2.73579266845179	-0.28959706830844	0.24850581504716
C	2.67092032766098	0.19863398361076	1.55161833270029
C	-0.13276429602753	1.50242517164012	-1.34260715162244
C	-0.89745309561081	1.81773219782448	-2.23456579938688
C	-1.76728590990620	2.20451494630487	-3.33086457159306
C	1.86413868209031	-0.34685481768728	-2.06036148438861
C	1.83431445531495	-0.71035892478455	-3.22083589461273
C	1.73785628920926	-1.08632192372304	-4.62427351023997
H	-0.01350256705670	2.27775463930237	1.22354866431157
H	1.63370367262645	1.51048402498947	2.92374438649153
H	3.39202882024498	-0.14361714627992	2.29376320135018
H	3.50213510801328	-1.00991353254990	-0.03609608354794
H	2.74439909954520	-1.08417162561228	-5.07756659455529
H	1.36976278031841	-2.12145525024936	-4.70839815169070
C	0.82337636019295	-0.15814618658593	-5.41193396470219
H	-2.81595496386111	2.22049470734249	-2.98926528669998
C	-1.43235674695239	3.54130933521650	-3.97677894391246
H	-1.71549769245344	1.42599708429905	-4.11379850238435
C	-0.32374149367168	-0.65398982267040	-6.03873718388616
C	-1.15269655868942	0.19587775442119	-6.77934251131014
C	-0.83527942483088	1.54953714602787	-6.90163132416883

C	0.30467510172148	2.05423192210508	-6.26823225290703
C	1.12297891555128	1.20686508057319	-5.52310635707317
H	-0.57265642878773	-1.71282016321472	-5.94677682001876
H	-2.04538147744178	-0.20411455938904	-7.26107441791808
H	-1.47872885653591	2.21683545298251	-7.47442085441263
H	0.54069106962298	3.11574481067861	-6.33861272659104
H	1.99786297493826	1.60601701233747	-5.00850415907764
C	-2.27893170752023	4.04309775197116	-4.97374425093258
C	-1.96620755430606	5.22530632939647	-5.64348713667891
C	-0.80103209509821	5.92766537735538	-5.31869592746647
C	0.03750149746802	5.44123268857816	-4.31414192857006
C	-0.27724957213902	4.25418343311959	-3.64695017136900
H	-3.18323121517198	3.49190967193193	-5.23866896013818
H	-2.63192047700543	5.60021748739333	-6.42173248177442
H	-0.55418237316051	6.85127249775913	-5.84196558908135
H	0.94449867275444	5.98526524753243	-4.04871443959540
H	0.38166811346873	3.86317888218801	-2.87112480857254

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Transition state

C	2.28461621529780	1.44344830900962	1.81858485562567
C	1.15783758913508	1.83162535177481	1.10572571735985
C	0.83686306353419	1.27219219188858	-0.14571591549252
C	1.75722812209083	0.23746527843277	-0.70024179189868
C	2.87841373768566	-0.12082068958818	0.07188124068543
C	3.14316628251365	0.46470188115783	1.30300640415179
C	-0.26546538685074	1.60299355579140	-0.92918503904105
C	-0.69986339653136	1.23963027455249	-2.07780192030853
C	-1.76529669985255	1.64713563171482	-3.03280673623542
C	1.41941024528297	-0.29165395269858	-1.94384739700568
C	0.45960682785715	-0.10837281803531	-2.77070393217247
C	-0.00413136901228	-0.62390769700799	-4.08618154606930
H	0.48995844692357	2.59167397103501	1.50754144976299
H	2.49591100398341	1.90354680704304	2.78332066476827
H	4.02487439493872	0.15841982685292	1.86548687355319
H	3.54693439346351	-0.88118822608323	-0.32791168092441
H	0.57975655548491	-1.53626845106750	-4.27991687259844
H	-1.05272317460099	-0.95179102318441	-4.02028588382119
C	0.15182211211907	0.32456730066329	-5.26240235050885
H	-2.67056368323322	1.83468430452325	-2.43349804933958
C	-1.43740676841583	2.89307848613109	-3.84483214445245
H	-2.02272089784671	0.84000360120201	-3.72860298171383
C	-0.61517161160683	0.12176704210394	-6.41665382734601
C	-0.46861029013224	0.95765766452655	-7.52446929701881
C	0.44540392590466	2.01349598908698	-7.48723567809238
C	1.20943385830299	2.22453813275884	-6.33826845889707
C	1.06441757775445	1.38363530527274	-5.23352058733243
H	-1.33663315927380	-0.69814967325684	-6.44606058410014
H	-1.07552243889163	0.78977456530743	-8.41465488350953
H	0.55173577149622	2.67674772717159	-8.34578223113957

H	1.91031957661834	3.05779615032322	-6.29290074596835
H	1.64881083894148	1.55696000376956	-4.32957036442358
C	-2.04631591772611	3.07155927068959	-5.09281932864005
C	-1.77654355933240	4.20398814267425	-5.86069707793208
C	-0.89240485129290	5.17701997956244	-5.38790727989592
C	-0.28617553361607	5.00792928156563	-4.14123283631025
C	-0.55695631579249	3.87261578909399	-3.37487950294792
H	-2.71658367787955	2.30135975686312	-5.47746832343864
H	-2.24474040583490	4.31693557771866	-6.83831707256389
H	-0.67149198561332	6.05707327816856	-5.99230969876524
H	0.40882379465186	5.75967743798561	-3.76528685727717
H	-0.06977621064463	3.73184066450641	-2.41017532872578

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Intermediate

C	2.26580384961131	1.45134255223065	1.79252526041620
C	1.14496364919535	1.85225015160942	1.09458147228294
C	0.82837413055986	1.29134713857745	-0.16854675842989
C	1.73163135531911	0.26483527102235	-0.72410574612770
C	2.86691687222056	-0.11195054069096	0.03685088294513
C	3.12819158572911	0.46509431402081	1.26281799251723
C	-0.26402978953092	1.61946585694542	-0.96298961395827
C	-0.59356243980879	1.12763795968244	-2.17998796101080
C	-1.77633021885096	1.63513179027164	-2.97527032752587
C	1.36962420514669	-0.24044208263983	-1.96807582805261
C	0.30091045921066	0.09306758863290	-2.72869930999162
C	0.01553981441019	-0.54558577176579	-4.06933321925883
H	0.47771591833188	2.61213749309358	1.50051352309286
H	2.48804958854458	1.89817114793585	2.76110567920700
H	4.00826940454190	0.15810313640988	1.82763792746061
H	3.53076671409796	-0.87216189892299	-0.37369416914699
H	0.69440605066098	-1.40416618361574	-4.17881861250891
H	-1.00443994047746	-0.96124822166368	-4.07374567926229
C	0.17574434176774	0.37452848255839	-5.26546629739085
H	-2.58154510599844	1.87969508389403	-2.26645722147519
C	-1.46629523761733	2.86512701194681	-3.81459979966350
H	-2.16327342081720	0.84642095721670	-3.63333163775938
C	-0.57505186115741	0.14746009277244	-6.42578180730687
C	-0.42338514992819	0.96500068248413	-7.54699778081371
C	0.47970668464654	2.02977910770088	-7.51836007821993
C	1.22894904263024	2.26719275862522	-6.36411369949545
C	1.07952740399651	1.44354155995256	-5.24775344220863
H	-1.29063293315808	-0.67764845204889	-6.44801218656248
H	-1.01908092896349	0.77610648612355	-8.44057052076289
H	0.58993879547981	2.67933323597027	-8.38685990316163
H	1.92161433858831	3.10768862713424	-6.32502985817078
H	1.65386630160676	1.64260516064427	-4.34274909549979
C	-2.05842610941603	3.01645874816333	-5.07402855913946
C	-1.79201868689465	4.13913164196644	-5.85821097984714
C	-0.92992568983568	5.13325253785966	-5.38966995886402
C	-0.34084053329604	4.99458106366440	-4.13066149578273

C	-0.60688974411277	3.86822651108944	-3.35051510055326
H	-2.71350490454101	2.23156597469394	-5.45468793308767
H	-2.24671657388515	4.22793948627552	-6.84461728060987
H	-0.71237182374108	6.00597253616335	-6.00581481022675
H	0.33650817643415	5.76322866949625	-3.75662036807108
H	-0.12866359069953	3.75423933451969	-2.37699469797516

$R_1 = \text{CH}_2\text{CH}_2\text{Ph}$, $R_2 = \text{CH}_2\text{Ph}$

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Substrate

C	8.90277316019580	-0.41634718792138	-5.18159724776933
C	9.24538075904974	0.84419862683003	-4.67610992485302
C	8.52238606895196	1.96043867195362	-5.12644979533324
C	7.49542380466315	1.82647981632670	-6.05859787777142
C	7.16486663998099	0.56242106453582	-6.55973169295517
C	7.87224778550519	-0.55629617242230	-6.11603292576547
C	10.35104415693529	1.06294283357834	-3.66642011987534
C	11.24351842873651	-0.15073731131506	-3.34410779088972
C	10.56096972074007	-1.21117718282677	-2.61625494905797
C	9.95589706973392	-2.08959899443953	-2.03041252558256
C	9.20600910705842	-3.11076412655172	-1.38970981091444
C	7.78113027749029	-3.02937683878095	-1.35286455639646
C	7.05460239225243	-4.05923821147753	-0.72695651195473
C	7.70641755293955	-5.14590093745796	-0.14905179538714
C	9.10324688440613	-5.22386475597807	-0.18225629224209
C	9.84324919248244	-4.21597886547801	-0.79546566501758
C	7.12365786128369	-1.91417188652422	-1.93490259873960
C	6.60550814112669	-0.93221898956955	-2.43214366830412
C	6.04201841307544	0.28063581030931	-2.99574055598197
C	6.58722611504483	1.57162761375791	-2.40076153494533
C	6.07236888483730	2.79457347059811	-2.85232555981486
C	6.57377260856973	4.00098105926446	-2.36635366117536
C	7.59821489833369	4.00172662117494	-1.41377562572655
C	8.10644218166523	2.78708153740093	-0.95108780270961
C	7.60345606777285	1.57800309523397	-1.44203790231880
H	10.93124356816049	-4.26837148964884	-0.82695989631760
H	9.61588357788092	-6.07230279679645	0.27092247506134
H	7.12511448716016	-5.93355567926299	0.33025550013007
H	5.96753420291086	-3.98833861357403	-0.70276715554895
H	4.94401054828826	0.26738713574534	-2.88732494235471
H	6.23781179512977	0.29494634253360	-4.08297531693580
H	12.10466017871002	0.19730351059447	-2.75168195451187
H	11.66577274296399	-0.56089795508145	-4.27753478685863
H	9.90210173213300	1.43365431487622	-2.73261143910185
H	11.00063344696713	1.87384317419144	-4.03123229054054
H	8.76425885877687	2.94704450245683	-4.72749142979969
H	6.94807379145370	2.70851540759916	-6.39147610708920
H	6.36163512226908	0.45183396057809	-7.28891865095585
H	7.61754672313078	-1.54790834763783	-6.49012836156826

H	9.42502345677716	-1.30492832255803	-4.83185794091084
H	8.00792853646401	0.62777869796535	-1.09312027772933
H	8.90065854917919	2.77636557892493	-0.20322945526906
H	7.99134275922062	4.94382812748425	-1.03198332801780
H	6.16559556353367	4.94388074149094	-2.73115551353595
H	5.28170298605897	2.79829714989792	-3.60532923666357

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Transition state

C	10.05876912209034	0.91171972691795	-6.33840402089827
C	9.42004655312209	1.19870602912276	-5.12358576299124
C	8.65560451686549	2.37032770713834	-5.02712985486662
C	8.53184306102826	3.23377111932604	-6.11680214161616
C	9.17220673970978	2.93767828301169	-7.32350248354772
C	9.93796411580169	1.77368115383132	-7.43081663728093
C	9.49493977841127	0.24449940976479	-3.96274105023608
C	8.34554193652127	-0.79185606856294	-4.02427748844199
C	8.37869851510658	-1.71932687807882	-2.86433300067989
C	9.19628037308883	-2.55243424236474	-2.33810691755596
C	9.18987094532817	-3.36371813894671	-1.20766153448102
C	7.96836614780142	-3.29647161355413	-0.35207208018074
C	7.93085115361717	-4.10724702316177	0.79834993743371
C	8.98346064266659	-4.94481234752555	1.14560446409353
C	10.12989694573731	-5.00676714481556	0.34289186297683
C	10.22301511952682	-4.23281466138186	-0.80657110320645
C	6.96189132328957	-2.42861870925490	-0.77201999348244
C	6.82138237273413	-1.63509239686044	-1.76722612234144
C	5.83569497575464	-0.64896293980668	-2.28425733063284
C	6.22988885058285	0.81134120771466	-2.13087293885916
C	5.55063020106190	1.78902239831510	-2.87118171450513
C	5.85813302588589	3.14154542808545	-2.71860666624957
C	6.86276749694695	3.53565059996785	-1.82963467978045
C	7.55106735414017	2.56682512141525	-1.09654877339666
C	7.23468191257108	1.21343046681664	-1.24403529203947
H	11.11411546177114	-4.28311995538303	-1.42956955089385
H	10.95538160274715	-5.66350236905010	0.61728771410908
H	8.91260323343228	-5.55313980709681	2.04697917280519
H	7.04006789180977	-4.05945032856956	1.42204761328531
H	4.90244872179585	-0.82493713379543	-1.72921693631418
H	5.59795109830230	-0.85222177501199	-3.33915057855659
H	8.43991628101582	-1.38300602294081	-4.94866814956449
H	7.39867992655724	-0.24922467970191	-4.09900419291189
H	9.41443713543062	0.79299389454771	-3.01438919897205
H	10.45165319176335	-0.29642801402293	-3.95227146943473
H	8.15407666946427	2.60510777529609	-4.08782316615630
H	7.93654922373027	4.14259616202876	-6.02133129699341
H	9.07879936839268	3.61238209796628	-8.17501495820865
H	10.44512620016430	1.53833122138796	-8.36690471867687
H	10.66039697891073	0.00461026300964	-6.42580379498817
H	7.77187129443955	0.45702641474692	-0.67185258244702

H	8.34149385964436	2.86388311614424	-0.40642070353765
H	7.11200488679660	4.59067750678675	-1.71589744995160
H	5.32008838266383	3.88811792124212	-3.30297345477830
H	4.77353241177765	1.48657422530237	-3.57660897504766

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Intermediate

C	9.99316785498461	0.76657936685915	-6.35065159807156
C	9.35372250945607	1.11529644972875	-5.15254235549017
C	8.63712624072175	2.31962489855303	-5.10008381442293
C	8.55980967781329	3.15395409269098	-6.21656286764249
C	9.19977639563201	2.79551687205731	-7.40646296232237
C	9.91885172106917	1.59889794997770	-7.46990108465579
C	9.37405671556782	0.19507285708683	-3.96247686465260
C	8.19688728995182	-0.80567331686767	-4.00632456884475
C	8.14710700588095	-1.66816513803384	-2.76693987424471
C	9.12304474011437	-2.54611857901186	-2.43731879590564
C	9.21108509091299	-3.35479944726395	-1.31128603007095
C	8.09219401730996	-3.23832855624370	-0.35343999472170
C	8.12568872881590	-4.03578685731555	0.81842877895211
C	9.17355111244507	-4.89961797104362	1.06540962261352
C	10.24402972464574	-5.01170262562134	0.14919520067456
C	10.26073667912625	-4.25970358559163	-1.00788965929422
C	7.09555642745424	-2.33497811573801	-0.70586469444133
C	7.02806388425319	-1.55683255065933	-1.81118497799582
C	5.88871961596334	-0.59623627277811	-2.07594994066268
C	6.27132311217018	0.87101788020872	-2.01011527609593
C	5.58559118676532	1.81166122133956	-2.79040798697310
C	5.89637353239083	3.17057516179300	-2.71261689630168
C	6.91112725099189	3.60921255241961	-1.85761989179929
C	7.60615277163803	2.67834756770730	-1.08191278037620
C	7.28702298702604	1.32054841774170	-1.15659107562521
H	11.08552022523674	-4.34513293042280	-1.71486163373324
H	11.06433602622499	-5.69826828944487	0.35899073940325
H	9.17605511167693	-5.50031519174599	1.97485481956458
H	7.29858872160489	-3.94818384791463	1.52239465888397
H	5.10101068783913	-0.79766346475051	-1.33499775875653
H	5.44410537389131	-0.80624226546637	-3.06110807089247
H	8.30433506383488	-1.44634239629902	-4.89403862685825
H	7.26386678005680	-0.24410939704554	-4.12945367881792
H	9.30054584826166	0.77984320185368	-3.03471922607700
H	10.31534069044377	-0.37279327654630	-3.91740706681171
H	8.13637700212607	2.60121035688399	-4.17304834233427
H	8.00158049859520	4.08885284540939	-6.15601726329986
H	9.14263514794525	3.44706707560209	-8.27893221258490
H	10.42556392037299	1.31493310746497	-8.39271794307888
H	10.55807954868653	-0.16632942784013	-6.40356017314408
H	7.83540327156889	0.59686370751853	-0.55280699278826
H	8.40491708353634	3.00985080571681	-0.41756802532896
H	7.16379041669555	4.66814779272108	-1.80256289401021

H	5.35286054214651	3.88603445747524	-3.33018545730355
H	4.80185366615474	1.47395106483536	-3.47196016366080

R₁ = R₂ = CH₂CH₂Ph

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Substrate

C	7.16242710829218	2.59657870653266	-5.18774189403548
C	6.18628828494433	1.68131992697965	-4.76576462484464
C	4.83600416445309	2.00664565335787	-4.94954293381106
C	4.46656218847458	3.21708738523921	-5.54279605853254
C	5.44699276708486	4.12090597997070	-5.95919396172776
C	6.79727412273970	3.80581928342357	-5.78050673814254
C	6.59746263218093	0.40245556769911	-4.08442108806945
C	6.91048988500013	0.63380302973629	-2.58278407857082
C	7.48346127714493	-0.53998188909996	-1.94516830017850
C	8.00225768055723	-1.53396002856083	-1.46982372915433
C	8.60974223442253	-2.68308809675998	-0.89747220197627
C	9.67468947079839	-3.35239514137171	-1.57155880229409
C	10.25861801771109	-4.48411905083984	-0.97030187606424
C	9.81178156955394	-4.95210845523567	0.26251557992288
C	8.76586176293895	-4.29724864538965	0.92271284797292
C	8.17327842916361	-3.17643346460007	0.34731906346972
C	10.13686071990263	-2.88745516294299	-2.83181111680539
C	10.53987555319486	-2.48573468812853	-3.90813007518513
C	10.97130835107106	-2.00537596879822	-5.21272910083758
C	10.10553203114796	-0.85013534044159	-5.78113449767968
C	10.35527810804942	0.49739998102544	-5.14667095042507
C	10.74494681988965	1.58554656446650	-5.94077199665362
C	10.96517076041559	2.84649796364974	-5.38000048011954
C	10.80408843797610	3.03760617556554	-4.00607723091858
C	10.42389898348360	1.95903425543122	-3.20248851131580
C	10.19834400898377	0.70204460646426	-3.76633485672889
H	11.07104511059250	-4.98846660044970	-1.49198121351327
H	10.27847132344176	-5.82967268997175	0.70899371935171
H	8.41317721251542	-4.66037925014693	1.88743128701463
H	7.35913204659790	-2.65922530764511	0.85355202278101
H	7.62004871815377	1.47440991546817	-2.50350736941126
H	5.99455297018962	0.95052181875533	-2.05941605535310
H	12.02408214857924	-1.68095568910383	-5.16349885146241
H	10.94198266709327	-2.84854311868150	-5.92329590507617
H	7.50126762531737	-0.00267522392898	-4.55854972552675
H	5.81274151388848	-0.36176656171902	-4.17463699465392
H	10.30352768055278	-0.77423409290297	-6.85995413999982
H	9.04612499476000	-1.13179395960171	-5.67450084431046
H	10.86768319657614	1.44274080533899	-7.01632874758008
H	11.26036863703981	3.67967495318410	-6.01823795706342
H	10.97106494445446	4.02030107594205	-3.56505840737985
H	10.29569464990552	2.09569917448810	-2.12798724398990
H	9.88927336074931	-0.12691783829826	-3.13123406927553
H	4.06647608371684	1.30138630237385	-4.62900633826112
H	3.41099095032712	3.45311346531252	-5.68301435014869

H	5.15909820294415	5.06395841341385	-6.42414478284592
H	7.57089573938751	4.50154814334979	-6.10653359965502
H	8.21744525364153	2.35514951745017	-5.05451992093481

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Transition state

C	7.95843095445674	2.95570869672131	-3.66074597367406
C	6.87118183707049	2.08603769289693	-3.49855921373673
C	5.72514320097770	2.29887586703665	-4.27890838418260
C	5.67041658414771	3.34756723389532	-5.19882533786768
C	6.76447246952381	4.20310589688016	-5.35344652014070
C	7.90895980938131	4.00518912577858	-4.57887855121787
C	6.96590685172233	0.89972539922089	-2.57280469500625
C	7.14085572043632	-0.41548455899713	-3.37999767885027
C	7.69849511333590	-1.53911171010937	-2.58251482608357
C	7.29489490059892	-2.54551178949207	-1.89908224640115
C	7.93411545899191	-3.53324296729747	-1.15398090232076
C	9.42542741239699	-3.45785743550799	-1.08825603282632
C	10.09677757588194	-4.44651641139819	-0.34330990743659
C	9.41802972316567	-5.46405920505125	0.31453757741916
C	8.02057520652172	-5.53467121199898	0.25307844019164
C	7.30297296000262	-4.58746663484469	-0.46577106636321
C	10.02523855269457	-2.40646051962754	-1.77707617997701
C	9.58083084902589	-1.43707352825999	-2.48846763113165
C	10.09091994332928	-0.29770073889353	-3.29432290423381
C	10.22749424323760	-0.61849352578437	-4.80744838185504
C	10.25457420398621	0.64341417564598	-5.63392434022953
C	9.18611453329677	0.96384096644971	-6.48263147050928
C	9.17273414229562	2.15943537896573	-7.20307169303430
C	10.23252439076706	3.06022154241116	-7.08250221239026
C	11.30494558500632	2.75455369819321	-6.23966242826105
C	11.31474795938415	1.55628609873944	-5.52322036155118
H	11.18309249018367	-4.39220502201088	-0.29355568943407
H	9.97946062557251	-6.20795908136403	0.87976602287009
H	7.48954242001969	-6.33410138880127	0.76965100704727
H	6.21656178130940	-4.64310683239438	-0.51151444711107
H	6.16774573611559	-0.73588529431966	-3.77377896972805
H	7.76661618214368	-0.20689760571137	-4.25445970200176
H	9.44812571828484	0.58254101812241	-3.18239434080470
H	11.06934596207874	-0.01313898089529	-2.88655115756516
H	6.06877931090393	0.80939260385706	-1.94327582643727
H	7.81613210221061	1.02400338766209	-1.88899262653297
H	11.13643647982767	-1.21870996435235	-4.95921660387581
H	9.38438230851547	-1.24724696983196	-5.12436897265721
H	8.35114673419415	0.26758454183579	-6.57975339563748
H	8.32653693737603	2.39214292309928	-7.84934975788269
H	10.22296795454611	3.99670709623660	-7.64035749257250
H	12.13934360186439	3.45031639571303	-6.14259957872048
H	12.15994340747245	1.32367506388580	-4.87260845884110
H	4.86474485491556	1.63666334368995	-4.16160270193738
H	4.76945863578297	3.49953698843018	-5.79419353379735
H	6.72461449466006	5.01956825580705	-6.07486618575725

H	8.77192786396952	4.65992182330457	-4.69764110824815
H	8.86007121641734	2.80547116246486	-3.06470555870485

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Intermediate

C	7.81249266825331	2.91874204710292	-4.27517577056681
C	6.90420867883111	2.20883964497716	-3.47626763156041
C	5.54752568341270	2.55714273793772	-3.53217642514219
C	5.10755002505132	3.59424970692735	-4.35803355957093
C	6.02270848117163	4.29693864959145	-5.14548440863345
C	7.37710253352244	3.95457841945092	-5.10221573293729
C	7.37568338366174	1.05724027997274	-2.62541333930376
C	7.49791768744167	-0.23819077234883	-3.46186310688758
C	8.10391373332697	-1.38448705885674	-2.68565496635823
C	7.37735963517961	-2.32261367018307	-2.03800040706825
C	7.83801278572612	-3.38773569314401	-1.27142746663978
C	9.30672655320674	-3.49654896050935	-1.14665952743482
C	9.83642994445506	-4.56039343258703	-0.37354454188421
C	9.00936531727084	-5.47439784467466	0.24778078751395
C	7.60545335320972	-5.37203313615041	0.12659316789615
C	7.03678791424099	-4.35513839549435	-0.61402888275031
C	10.03988900585474	-2.52371870919187	-1.81812381376832
C	9.57311139539985	-1.49534227061421	-2.56095086226522
C	10.45267705705561	-0.49806744955467	-3.27648306364791
C	10.55056261938210	-0.76159468150923	-4.80880801858419
C	10.50662191819927	0.50382876774313	-5.63033332083822
C	9.55797736817118	0.66057986002977	-6.65002902302162
C	9.47460861128631	1.84721741163855	-7.38189006385029
C	10.34277653878517	2.90396070249099	-7.10217351458806
C	11.29503517778525	2.76274351416260	-6.08824223980426
C	11.37589209539990	1.57324181653658	-5.36162756542123
H	10.91953469198809	-4.63747225626516	-0.28115629403876
H	9.44336645310107	-6.28249851415760	0.83684046959154
H	6.96631356226730	-6.10228763831406	0.62287322941017
H	5.95407783029160	-4.27410949085454	-0.70856886816345
H	6.50013764306236	-0.52951227765800	-3.81467827915275
H	8.09481121257753	-0.01588532091916	-4.35624311695726
H	10.06401332979234	0.51591304952471	-3.11466740204629
H	11.44972856601283	-0.52295741948312	-2.82159456240058
H	6.68503096582417	0.88132381039864	-1.78889170902827
H	8.35435631336499	1.29733118908350	-2.18504012025701
H	11.47766312161140	-1.31972871173565	-5.01194477852796
H	9.72992903199359	-1.42058476555486	-5.12214281325824
H	8.86675457289861	-0.15680864332071	-6.86408124121337
H	8.72008521192102	1.95046249262363	-8.16193123700519
H	10.27705360320653	3.83352385732437	-7.66789299043186
H	11.97714803939592	3.58291604651564	-5.86136529592658
H	12.12157218129494	1.47661195300106	-4.57057370969907
H	4.83060108161813	2.01145922560793	-2.91527067808701
H	4.04920636154563	3.85648220696485	-4.38356235577047
H	5.68196862314486	5.10940489695223	-5.78803659758270

H	8.09981470654958	4.49265373378363	-5.71554507686535
H	8.87202483125607	2.65645889273919	-4.25515947547235

R₁ = R₂ = CH₂OPh

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Substrate

C	5.29086655490106	2.82633242377626	-3.21595095860036
C	6.39800083288491	2.63440117115821	-2.37868531751303
C	7.17348187362647	3.73443865170781	-1.98125718051512
C	6.85156364203750	5.01078729933093	-2.43193286752611
C	5.75305474225141	5.21191304717176	-3.27743015239980
C	4.97895847907200	4.11643330709193	-3.65800581286147
O	6.81397790137605	1.41953252464651	-1.90538037692961
C	6.14551728693522	0.26233381105191	-2.44126266862658
C	6.78725668685450	-0.93399177972443	-1.93417777937647
C	7.31207236011364	-1.95240689472526	-1.52805070576588
C	7.96430997442779	-3.12794075543560	-1.07428950576356
C	9.33441551624230	-3.35327928203700	-1.40201590867894
C	9.96598190695137	-4.52465804451298	-0.94596449559638
C	9.26729195705917	-5.45971761628195	-0.18677740126603
C	7.92393440290391	-5.23942564314715	0.13699341354972
C	7.28154205500214	-4.08405949090182	-0.30020524371526
C	10.03620915673989	-2.39792487595206	-2.18086045272384
C	10.60026011447049	-1.55959715438570	-2.85814127444432
C	11.24465152581312	-0.54157363056943	-3.67622488781310
O	10.54060157877140	0.70942141401783	-3.71428332502837
C	9.40023796872360	0.77663710379226	-4.47857791412624
C	8.87610893352446	2.06475037236707	-4.66121033267273
C	7.73452283905576	2.24772812390343	-5.43415637835794
C	7.10048744544245	1.15253247169185	-6.03342642743191
C	7.62169558070120	-0.12759306307944	-5.84041854587298
C	8.76786840597113	-0.32849672574052	-5.06272911609827
H	11.01255424127568	-4.68722024297423	-1.19959656195081
H	9.77172853017606	-6.36263369299434	0.15631633018923
H	7.37784665220996	-5.96990918060171	0.73369118390646
H	6.23780363389503	-3.90077487523953	-0.04922786314641
H	5.07966015938901	0.27610497145464	-2.15033946573508
H	6.20497680636247	0.28287113768133	-3.54443229519305
H	12.23196977597540	-0.29065516617861	-3.26403142634202
H	11.39512856404221	-0.91445927928003	-4.70561222452424
H	9.37337078593704	2.90687444496960	-4.18289966006920
H	7.32901378726945	3.25143839632206	-5.55510790908253
H	6.20512586076709	1.29811064045795	-6.63698859426993
H	7.13167261766012	-0.99175015839671	-6.28970944102421
H	9.13434845012404	-1.33854741636997	-4.89480156526232
H	8.03124717128603	3.55818877731493	-1.33276676266787
H	7.46615148803071	5.85688131050455	-2.12371210202637
H	5.50502706274284	6.21178193158054	-3.63121132552756
H	4.11895092154580	4.25744858257110	-4.31363594212914
H	4.68229886945817	1.98804355396403	-3.54555215899037

Transition state

C	5.71864833947201	2.04011405353692	-3.64343450500963
C	6.43125208036676	1.94447876654261	-2.44065913913156
C	6.80658369513629	3.10965805928635	-1.75467788549935
C	6.48429238663740	4.35745691426396	-2.27819889652029
C	5.78797439578392	4.46346064934060	-3.48800235797569
C	5.41049240618400	3.30231088960635	-4.16002685134346
O	6.82252115338384	0.76865461015827	-1.85262796436160
C	6.51192532267604	-0.44476855641102	-2.55024278547671
C	7.27518470773834	-1.55990393595746	-1.94206229259855
C	7.20030988822196	-2.34245804668045	-0.93419586149544
C	8.01138861116493	-3.33792382984985	-0.39471549427580
C	9.27629964671100	-3.63556586999432	-1.12658641005548
C	10.11243181728677	-4.64024074889709	-0.60551884157992
C	9.79148128039928	-5.33755209849672	0.55177225291809
C	8.60793879755704	-5.05198140834450	1.24304864218895
C	7.74146571615335	-4.07307912173790	0.77443769924661
C	9.52646369873727	-2.88392511176101	-2.27388259760477
C	8.89140991499177	-1.96263340685624	-2.89181558033678
C	8.98667901924694	-1.16186897992630	-4.13389681025295
O	9.22125936815081	0.21007685021658	-3.79908688190353
C	8.92485322950267	1.16138888844214	-4.74549345810098
C	9.07282551210408	2.48972325658267	-4.32000304031888
C	8.74918591557685	3.53184781785043	-5.17915110884163
C	8.28175601721401	3.26966509441481	-6.47343042574625
C	8.15630090148161	1.94921557076747	-6.89732906739338
C	8.48054868341312	0.88579584244162	-6.04438888864869
H	11.03387434055396	-4.86099356581567	-1.14073510393381
H	10.46850321190283	-6.10774342648926	0.92083526319164
H	8.36113205151539	-5.59758709268283	2.15327732017519
H	6.82201810518007	-3.85169625426433	1.31273763575902
H	5.43534573113783	-0.66368014346075	-2.45396039721868
H	6.73712279442899	-0.32689054665916	-3.61787525014812
H	9.81645970096882	-1.55269808663741	-4.74335278157504
H	8.06201231304803	-1.25878474791427	-4.72578731107251
H	9.41144049309299	2.67554534166037	-3.30273749918984
H	8.84381248790524	4.55905492407653	-4.82852459629534
H	8.01955628152853	4.08989189746337	-7.14041042034548
H	7.80664559643566	1.72819902430432	-7.90604047962352
H	8.39136238896731	-0.13533621072453	-6.40980172696415
H	7.35765456927333	3.00765075625934	-0.82064669274864
H	6.78346703079229	5.25660241126424	-1.73907414550923
H	5.54390567225074	5.44202211146970	-3.89941942534893
H	4.87254414014979	3.36815150468607	-5.10558812762149
H	5.41234558557612	1.15387095492637	-4.19340271141339

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Intermediate

C	5.70037426120799	2.08511834618977	-3.54320430308574
C	6.53126026296471	1.96521895426581	-2.42177201100516
C	6.96597734627249	3.11629849317333	-1.74630059015669
C	6.58787965070792	4.37425343308177	-2.20309078856277
C	5.77456907157525	4.50511057777420	-3.33513031302936
C	5.33715529734062	3.35767953317831	-3.99470400068194
O	6.99012708800728	0.77927120603833	-1.91115734901017
C	6.62556621885258	-0.42508728525495	-2.60020281569984
C	7.51651449211058	-1.53577459169634	-2.10710864793175
C	7.28004205418953	-2.22100971535928	-0.96618338547507
C	8.04838441632497	-3.23620143618382	-0.40567345346415
C	9.26199232450998	-3.61023660315790	-1.15804568184612
C	10.08441287551650	-4.63970423035127	-0.63615523096972
C	9.76393520165389	-5.27857467355495	0.54424397361011
C	8.60367101962667	-4.91916172549900	1.26544128312117
C	7.76821830558281	-3.92363395121311	0.80169757457534
C	9.48654343335584	-2.89840264707459	-2.33253948825852
C	8.72318853317320	-1.91591224822530	-2.86072122068004
C	9.02614083903393	-1.24074057177455	-4.17314888117718
O	9.35426234033463	0.13221684439556	-3.92401222978762
C	8.94593189530948	1.08736750409860	-4.82256415063712
C	9.08656536922811	2.41347972811945	-4.38654936193798
C	8.66436544623142	3.45997400153971	-5.19714437933129
C	8.10160085895310	3.20513273589801	-6.45371054495094
C	7.98317696008993	1.88821049998343	-6.89127408242980
C	8.40804282303706	0.82182982967506	-6.08841448120779
H	10.97944954029385	-4.91454508514876	-1.19274466523458
H	10.41255640067377	-6.06757699652087	0.92465375686346
H	8.36713291626051	-5.43228453316704	2.19710031888575
H	6.87386177641828	-3.64285461373780	1.35647843997152
H	5.57072430690383	-0.66443132689787	-2.39022727244539
H	6.74026872123653	-0.28403949348281	-3.68504396372437
H	9.86876848205866	-1.74172703989569	-4.67071009088098
H	8.14659884054704	-1.30966791064418	-4.83115304788274
H	9.49835107672336	2.59362234253951	-3.39557636319626
H	8.75345528624972	4.48320834008532	-4.83380949267112
H	7.76080527089053	4.02732929661170	-7.08138357960681
H	7.56231911620092	1.67302288505006	-7.87366538156159
H	8.32803806818676	-0.19462859890834	-6.46929780959891
H	7.60917532077480	2.99535039979786	-0.87516611961136
H	6.93528948412302	5.26185011298977	-1.67382583380929
H	5.48610982843190	5.49154388110759	-3.69599720520725
H	4.70633545680562	3.44323621510265	-4.87971106960805
H	5.34699942203042	1.20852841705267	-4.08034436067189

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Substrate

C	-0.17756891188427	4.27646267602515	-4.24964015548668
C	-1.40311949149409	3.62654791386881	-4.08035596312308
C	-2.56728903105719	4.34341468745978	-4.38710399690413
C	-2.51153493823619	5.65854907566648	-4.85083466166498
C	-1.27988654482062	6.29495460477880	-5.01923993618686
C	-0.12040433199036	5.59264342942039	-4.71474987282202
C	-1.47211569789327	2.18023467773032	-3.62817885951167
C	-0.75652597096380	1.87478362220216	-2.39940924775871
C	-0.11316782249896	1.56344549352606	-1.41641675653012
C	0.71615743863479	1.09650321308286	-0.36479696411776
C	0.60456008307325	1.58383841572517	0.94941769596716
C	1.42851854613153	1.09833515318526	1.96220689763925
C	2.38083645579714	0.11241894378548	1.68041355051873
C	2.51200500416388	-0.38273901160100	0.38479916449649
C	1.69353074927404	0.09525526927043	-0.65435309246104
C	1.81725010164073	-0.39320777005534	-1.98193761179764
C	1.87665211328478	-0.77184270775663	-3.13629025503451
C	1.92078399838477	-1.17497900357564	-4.53623060597443
C	1.06203237515160	-0.28265131939612	-5.41896687364701
C	-0.17898847628338	-0.72150394698420	-5.88214830525355
C	-0.97246477118492	0.09175853063061	-6.69859583723377
C	-0.54464224106129	1.36102801945282	-7.06669822091464
C	0.69430880621823	1.81367959172825	-6.60317012459678
C	1.48229278576150	1.00237434162275	-5.78819656525666
H	-0.14109069506253	2.34964822454859	1.16034087664070
H	1.32763342059264	1.48818066070180	2.97484710737216
H	3.02292125127829	-0.27116937913033	2.47297172978439
H	3.25176949352769	-1.14942680938233	0.15652222769051
H	2.96039147493897	-1.13653665654776	-4.90102482884374
H	1.59417501134947	-2.22075842712602	-4.63483668307877
H	-2.53269984321873	1.90253289274839	-3.52724873919946
H	-1.06132750243086	1.53827345252376	-4.42594716732317
F	-0.63870537921934	-1.94991336106053	-5.55044558794147
F	-2.16801913667615	-0.37660441709650	-7.12189219848133
H	-1.18539676576081	1.97610192456443	-7.69677988983158
H	1.03767898214328	2.81056125804540	-6.87287247826249
H	2.43734595743428	1.36963907995083	-5.41460968531646
H	-3.53138893765346	3.85138796952514	-4.25692786642102
H	-3.43120544589439	6.19408852346693	-5.08173080804959
H	-1.20125614372577	7.31960232529796	-5.37844059684026
F	1.09099133434186	6.17369524272328	-4.87274763497735
F	0.98182769588815	3.64170459645455	-3.97741617926663

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Transition State

C	-0.87658348143298	3.78077250497594	-3.94592332723617
C	-1.84276703867806	2.79274792747568	-3.74343612586115
C	-2.72564269938811	2.52385476039154	-4.79943576494406
C	-2.63906337945901	3.20036449895358	-6.01508616638666
C	-1.65314333604808	4.16951199237451	-6.21026963820869
C	-0.77931829685619	4.45018121452433	-5.16888863654889

C	-1.97821525982357	2.04887808752059	-2.43002511454172
C	-0.73748531852993	1.57816926345770	-1.74527399481544
C	-0.12422957962839	1.77219492852485	-0.64077706392239
C	0.98837667798140	1.21972806183628	-0.01331703166646
C	1.49718532893162	1.59596954034274	1.24427653046015
C	2.62202977441689	0.99381998344381	1.79351651211706
C	3.28870846357241	-0.02316321383213	1.09890370487997
C	2.82829416355445	-0.44083659041150	-0.14338293805109
C	1.69306898637737	0.13020932214219	-0.74916980889020
C	1.16788644154844	-0.21885148372637	-1.99135515738751
C	0.19081441696084	0.19981539199580	-2.70392631924631
C	-0.34322781057802	0.00023011849470	-4.07451471507956
C	0.32903987259295	0.86631376372031	-5.12624292551751
C	-0.22092346023005	0.91603519930561	-6.40761145807413
C	0.34292141030989	1.70838880243755	-7.40699282238220
C	1.48294376912367	2.46096217100411	-7.15554952383277
C	2.05045469337994	2.41117825849866	-5.88066382567806
C	1.47894677328055	1.62513315114274	-4.87961066402649
H	0.98068484672758	2.38718809008473	1.78428361038711
H	2.98401947115570	1.31900514718450	2.76815260875321
H	4.17301237697073	-0.49156565880151	1.52975157438529
H	3.34827091281717	-1.22967063577608	-0.68361162159804
H	-0.19455822122392	-1.05991569151431	-4.33238768589849
H	-1.42739600734979	0.16431872714785	-4.12303075719891
H	-2.48690486832907	2.69952280345803	-1.70324790031526
H	-2.65296175998456	1.19589675289666	-2.59779808226584
F	-1.33102062629476	0.19093383416321	-6.69356935854905
F	-0.25004450063041	1.74613897199471	-8.62326411423960
H	1.89825221626741	3.07746420074064	-7.95101503754120
H	2.93918345727651	3.00161795781702	-5.66474208111811
H	1.91137960465683	1.60128144887251	-3.88045631103509
H	-3.48480513548650	1.75255633972213	-4.66296115765722
H	-3.32611088591788	2.95798042649392	-6.82422108813550
H	-1.54232313440620	4.70021235521806	-7.15430829951347
F	0.18824000047244	5.38022805389250	-5.32289972309573
F	-0.01009885809930	4.11155722181222	-2.96658530052385

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Intermediate

C	-0.86287184917075	3.76810470510256	-3.92895587925698
C	-1.83528369758627	2.78643638073466	-3.72502909668055
C	-2.72090446519861	2.52615087004693	-4.78044698548464
C	-2.62985024633369	3.20504445209592	-5.99501236439753
C	-1.63851516430244	4.16890134617246	-6.18889599435610
C	-0.76169109777098	4.44251336408403	-5.14754138153537
C	-1.94119986261060	2.03815028640065	-2.41483532135484
C	-0.66462068281606	1.41190746819664	-1.87735445738078
C	-0.18257586872908	1.71163658462885	-0.64776930201504
C	0.94086312098551	1.19573672591873	-0.01212798950329
C	1.41494510804849	1.55604950466689	1.27509100569736
C	2.55241223660049	0.97893603267958	1.80175594833582

C	3.27392522823013	0.00900173592472	1.06866334217085
C	2.85409623252864	-0.37927158703735	-0.18723510857078
C	1.69276760768298	0.18315276100116	-0.77585231522223
C	1.17940547753953	-0.11772968684926	-2.03243112055779
C	0.08802195405866	0.40645817623788	-2.64097166881978
C	-0.31567112638000	0.02069790958692	-4.04547400244086
C	0.33868757638032	0.87003884099061	-5.12078008115354
C	-0.22026548880363	0.89912770770639	-6.39932560880827
C	0.33465305060844	1.67575498466456	-7.41661469018926
C	1.47724473911135	2.43160850101000	-7.18953133139344
C	2.05627176816042	2.40196580674594	-5.91913122926646
C	1.49235894342293	1.63384305500255	-4.90029776706348
H	0.85805095327691	2.30491459109290	1.83724925305274
H	2.89881219912106	1.27398287754659	2.79167625330379
H	4.17118755078317	-0.43463227051887	1.49913529857705
H	3.40949609328771	-1.12472662840683	-0.75537425829751
H	-0.04116616993193	-1.03228824716821	-4.20922463092406
H	-1.40555990709777	0.07390330199369	-4.16503114626831
H	-2.31799123078814	2.71641161128634	-1.63588872990684
H	-2.70299802876557	1.25314246990965	-2.53894736544545
F	-1.33165572425133	0.17032062158666	-6.66891937542713
F	-0.26970623163560	1.69331993353949	-8.62781220544489
H	1.88527670147071	3.03460200078741	-7.99895771852302
H	2.94737264953741	2.99499245414794	-5.72059786727844
H	1.93747962840424	1.63198771307800	-3.90641226367928
H	-3.48403159676765	1.75885307840697	-4.64492838713587
H	-3.31899517628549	2.96946327526290	-6.80447845525867
H	-1.52598928726943	4.70155088556229	-7.13165827252045
F	0.21184516092091	5.36719464000710	-5.30038547360427
F	0.01020392233502	4.08102576617398	-2.94636325597245

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Substrate

C	1.97736344867004	1.48571270889449	-5.35504227637301
C	0.70469038155091	0.96807835778967	-5.60492917421357
C	0.17908875912980	1.00934653826685	-6.90890294354411
C	0.95294057368421	1.55738757941752	-7.95685842845314
C	2.22031031770431	2.08018886310140	-7.68240313399796
C	2.73135283459349	2.04930407941274	-6.38391164936952
C	-0.16089062765248	0.37526915649104	-4.50661371596093
C	0.43395339392877	0.37506016423965	-3.18332033381967
C	0.92146235525535	0.37463123876332	-2.06885380498898
C	1.38959614773771	0.46101327507393	-0.73212690131676
C	0.71200302854096	1.32195006677975	0.18574420118367
C	1.16964125294955	1.40930710087420	1.51207024589196
C	2.27295069690858	0.67067563650673	1.93384649100045
C	2.93933968673454	-0.16979903366823	1.03530787117182
C	2.50068622032678	-0.27441767109152	-0.28296755797252
C	-0.39746678066308	2.07269129163107	-0.28418571703299

C	-1.31945910778918	2.66328781408702	-0.81691461194831
C	-2.35590965037697	3.38148933325931	-1.54979953323049
C	-2.20053683932104	3.30308666895140	-3.06154749574509
C	-1.03657400130522	3.79178928645416	-3.68527652094482
C	-0.96665985544010	3.82884544435556	-5.10249073564602
C	-2.01389456858584	3.30076332425343	-5.86038609114076
C	-3.13699887959647	2.74803275873940	-5.23686706005238
C	-3.23228462631280	2.76924157189140	-3.84422054659928
N	0.04664341848080	4.30360179848667	-2.96588363854503
N	0.20595896809261	4.34251240969610	-5.67641305666350
N	-1.07995030747304	0.47151084396820	-7.22231325511803
N	0.37038672745796	1.60682343004089	-9.24808886314710
H	0.64604092413312	2.06849054105188	2.20365536924067
H	2.61610937523374	0.75134761381769	2.96504664402007
H	3.80460009514555	-0.74515234741281	1.36416503912356
H	3.01277014234965	-0.92858593929494	-0.98777440802192
H	-0.43534115438602	-0.66058782031329	-4.77798209474838
H	-1.11325529206357	0.93712528153862	-4.45239495510572
H	-2.34754124256228	4.44067641571892	-1.23456868863859
H	-3.34593735465004	2.98800612525503	-1.27222711899523
H	2.81095800736366	2.49935584759701	-8.49984381003157
H	3.72100897063032	2.45528961051992	-6.17866214487511
H	2.36492860563524	1.45038262549897	-4.33682327956257
H	-4.12263136878026	2.37765420531810	-3.35002662385404
H	-3.95086471430137	2.34024659947438	-5.83631409289960
H	-1.94234054660720	3.33149377508460	-6.94901660412097
H	-1.51556207743695	0.96373260345442	-8.00245981782301
H	-1.72220400772122	0.46250848441449	-6.43233324752444
H	1.02715943116914	1.93634282106298	-9.95219700848322
H	0.00103453257562	0.70075241892032	-9.54039238621660
H	0.92006587057952	4.18275634721879	-3.48206448879424
H	0.12851222090290	3.91105539401733	-2.02778228938808
H	0.24045862659569	4.27808625571301	-6.68952060379083
H	0.46324298896444	5.27135810467837	-5.34861115293398

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Transition State

C	1.40545936048727	1.70885763337992	-4.83534761932633
C	0.32727845475801	0.87124848985064	-5.13256209661162
C	-0.19636442506520	0.83803050076728	-6.43851553205270
C	0.36607381108334	1.66787294100804	-7.43561690452065
C	1.42254451465938	2.52009684428459	-7.10637935939792
C	1.94386549856966	2.54295926796549	-5.81276221582844
C	-0.35137286707227	0.00960811660671	-4.08384765904110
C	0.16245277374741	0.20159088833549	-2.70541993439090
C	1.10692510105402	-0.23858576604356	-1.96361023734797
C	1.64686305128848	0.11876102139608	-0.73144686647894
C	0.98843537746238	1.25732824386371	-0.03033807014630
C	1.51091521406278	1.64707977414023	1.21766590410755
C	2.60850808139833	1.01382003365463	1.78736229370766
C	3.23269592332692	-0.04960765717027	1.12302453435765

C	2.75677094390602	-0.48281279367621	-0.10820870367524
C	-0.10505329903767	1.83707802114986	-0.67251964759209
C	-0.72313006992719	1.61427997596835	-1.77431474325684
C	-1.95971316959048	2.09994760509201	-2.47107410090704
C	-1.81859771437752	2.85339654646055	-3.77912953661701
C	-0.88808641998536	3.89562706254790	-3.94515320766926
C	-0.82065182365596	4.57505318173649	-5.18722360924533
C	-1.65428708797098	4.19278533630058	-6.23881078864115
C	-2.57899619118315	3.16180722790822	-6.07015937559640
C	-2.66383058475126	2.51001293459568	-4.84396382705218
N	-0.03656299895513	4.34899934369795	-2.92674088932006
N	0.14989225154514	5.58753513268621	-5.32188551045683
N	-1.31737767230686	0.04932607329737	-6.73119376714359
N	-0.21214573078052	1.65531113474071	-8.73099573907571
H	1.02485796286844	2.47195406152420	1.73528073175246
H	2.98162629480078	1.34940321136515	2.75429893705456
H	4.09545044656668	-0.54319911499426	1.56953288359462
H	3.24444116892731	-1.30721269445920	-0.62485410216285
H	-0.20804554599911	-1.05986872636011	-4.31662070844498
H	-1.43508708156589	0.18820313865490	-4.15175171066843
H	-2.46603801172959	2.73723515405591	-1.72941323388870
H	-2.63086040450886	1.24517301130313	-2.64144044420380
H	1.84486762224894	3.16394507578523	-7.88053727122484
H	2.76688684652192	3.21406003563990	-5.57126504964687
H	1.79777011446926	1.72079288987819	-3.81937933764096
H	-3.37322065962555	1.69172269082856	-4.71232712371750
H	-3.21513517092270	2.85883692569228	-6.90033487548290
H	-1.57476968547926	4.70945368309785	-7.19741196111485
H	-1.67348498211334	0.13567055036071	-7.67621995309668
H	-1.31116593970435	-0.90608316600800	-6.39139280998331
H	0.28685523719559	2.26669788266373	-9.37384645154341
H	-0.24666793016981	0.71835827172536	-9.13706124250865
H	0.89404016142452	4.56815665265872	-3.28500681072865
H	0.03326456230597	3.71601720422215	-2.12969641608662
H	0.03473752080536	6.13111996683175	-6.17335768600611
H	0.18241517099410	6.20666518098917	-4.51077215503274

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Intermediate

C	1.37945480514495	1.76621058181843	-4.88172736624099
C	0.31335587386839	0.90096110093811	-5.14625591377647
C	-0.19658254331809	0.80549674201161	-6.45561558569709
C	0.36927440268969	1.59228138359218	-7.48539981576875
C	1.41565637121694	2.46810083219710	-7.18807868878005
C	1.92144523683586	2.55894843019402	-5.89112922415677
C	-0.35412311030844	0.07139110009141	-4.06570326977751
C	0.05265103381655	0.43854950269725	-2.65893961447158
C	1.13020824593536	-0.10378365426283	-2.04510094508236
C	1.65580425046143	0.19553989028958	-0.79381399734511
C	0.92607480474373	1.22748605379860	-0.03202690382472
C	1.41182090968924	1.58496347031553	1.25123170846722

C	2.54067194347695	0.98958124461544	1.77736534677936
C	3.24204686938534	0.00417548572760	1.04604798634583
C	2.80964073665058	-0.38288459085101	-0.20635203245490
C	-0.19083240342673	1.75838522929300	-0.66846932245296
C	-0.69042069283555	1.45342030476502	-1.89069591685023
C	-1.96033101691286	2.09957113403358	-2.43404851513026
C	-1.82867346769087	2.86986464309132	-3.73051574242839
C	-0.88795195642562	3.90598650148297	-3.87358672177406
C	-0.78202546591363	4.58748188337070	-5.11036850226856
C	-1.58656705829766	4.20755661813197	-6.18535408372848
C	-2.52252859240067	3.18282076264963	-6.04184148118974
C	-2.64721876792736	2.53313095444907	-4.81760063659046
N	-0.05623044148063	4.34449370832341	-2.83070755485476
N	0.20334619839436	5.59008740236409	-5.21868519797338
N	-1.30696745696808	-0.00286655745144	-6.72545432302851
N	-0.19724941477387	1.51238256302224	-8.78448242292435
H	0.86901510447903	2.34426938801436	1.81331858485498
H	2.89488814345894	1.28202952953684	2.76535546696000
H	4.13333532694508	-0.45321631484622	1.47471311918384
H	3.35033696081879	-1.13975219165874	-0.77356946966366
H	-0.11916029181577	-0.99668375522063	-4.21420630461961
H	-1.44367268042541	0.16962285570768	-4.18612533873611
H	-2.35093519851810	2.75084423167940	-1.63702152008623
H	-2.71320484117280	1.31063751639045	-2.58307686271530
H	1.84175685879641	3.07545572770685	-7.98925894762051
H	2.73241255772090	3.25147103617139	-5.67063129647711
H	1.76303207345760	1.83568850164201	-3.86472713475846
H	-3.36482741513995	1.71912998344320	-4.70489634974559
H	-3.13630653437951	2.88258632650738	-6.88967104073748
H	-1.47506005787015	4.72126168067787	-7.14234101655455
H	-1.64628684475358	0.01755721534711	-7.67964102411000
H	-1.32481971772586	-0.92475948500843	-6.30519388453586
H	0.29991873872204	2.10147132893677	-9.44936695910981
H	-0.21025114288763	0.55732935120779	-9.14791532024390
H	0.87952341331046	4.57549724992705	-3.16773960606709
H	0.00494485597297	3.69820734259647	-2.04507136283735
H	0.13120557304695	6.11796006063705	-6.08468860808377
H	0.20282182433024	6.22607569990574	-4.42011738731839

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Substrate

C	1.60451084449318	1.74892989929303	-6.18974672559422
C	1.27452711148493	0.58657188492216	-5.48170943403447
C	-0.04799753574291	0.14570859872654	-5.53427697825409
C	-1.00832780174505	0.84127953053441	-6.27189482994012
C	-0.67684816041526	1.99744917742716	-6.96382189915098
C	0.64213878567279	2.45012496250999	-6.91800705493339
C	2.30412219452439	-0.16939571808327	-4.66059760756308
C	2.13042797792962	-0.00023427123698	-3.22104567081567

C	1.95530003309675	0.12297120484893	-2.02273921624972
C	1.73101503053229	0.26931310535147	-0.62669171789818
C	0.53242319297627	0.88712832360027	-0.15473486179868
C	0.33057695170433	1.01807488566703	1.23075707178060
C	1.27915968163570	0.55145917666603	2.13747984876156
C	2.45223049487823	-0.05614824966170	1.67589237593143
C	2.67472136351334	-0.19488230159446	0.30809569350622
C	-0.41852233394401	1.35809789485469	-1.09594097526021
C	-1.14942780180396	1.72401702000783	-1.99788521711233
C	-1.97508064752628	2.13158797652068	-3.12294180784362
C	-1.55271622758659	3.34774438381655	-3.94625287547635
C	-0.23366486428633	3.82776351398655	-4.05694034464896
C	0.02711499176155	4.93103194506903	-4.91661570494947
C	-0.99495855513106	5.49171801432563	-5.68206942912505
C	-2.29678362915726	4.99470032147311	-5.58617614309988
C	-2.56653984742291	3.94636552212517	-4.71122178396948
N	0.86876835831208	3.33296019035271	-3.35056194239520
N	1.36078079610108	5.37269539942278	-5.01065052916335
F	-0.41716496346626	-0.97037818388984	-4.86374465313804
F	-2.28090173098221	0.37791876555909	-6.28328524736919
H	-0.58427266329363	1.49357550328367	1.58171566743113
H	1.10459226119383	0.66295509032176	3.20770424683277
H	3.19511084224857	-0.42230653897227	2.38411515930626
H	3.58503040124734	-0.66635618835142	-0.06012386902468
H	3.30641541764829	0.17502926424281	-4.95829915102263
H	2.25890125396205	-1.24446024179817	-4.90177202020387
H	-3.00052852278503	2.31212232986578	-2.76249074244319
H	-2.05924556265367	1.26326526446664	-3.80129986142112
H	-1.45604159817824	2.54280172217347	-7.49206141255833
H	0.91554013286308	3.36849100594009	-7.43251542199265
H	2.63220510860346	2.11266736630326	-6.15831905460350
H	-3.58364059212631	3.56146747089398	-4.62312294460203
H	-3.09811280733065	5.44031021251701	-6.17441944503980
H	-0.76976605711775	6.33261648786264	-6.34106994441398
H	1.69502011369484	3.24561256072509	-3.94139542253676
H	0.69835736997899	2.47012928432734	-2.83861995933606
H	1.44509573579290	6.28244230649551	-5.45692592215627
H	1.82889545684549	5.37567712710798	-4.10322124241134

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Transition State

C	1.43398421849069	1.69459612714640	-4.87530599693430
C	0.34416302309013	0.86498434728790	-5.15131626740312
C	-0.21132035665485	0.84484817563187	-6.44523004729177
C	0.33671917270842	1.67111216268141	-7.45310534296322
C	1.41120246668896	2.50976426809546	-7.14622257234907
C	1.95919323276916	2.52584525159115	-5.86322651057486
C	-0.30986894697817	-0.00196220638153	-4.09081627949184
C	0.21515149917453	0.19765848160887	-2.71675319395956
C	1.18460518100839	-0.22413797594784	-1.99550161589210
C	1.69882169078773	0.12001411884942	-0.74784517694768

C	0.98727030765921	1.20638888333819	-0.01377452096059
C	1.48546915190567	1.57787158331840	1.24966229193948
C	2.60543172091736	0.97390323426393	1.80689107712704
C	3.27834800469117	-0.04037368502957	1.11408067523758
C	2.82901872657176	-0.45286817712194	-0.13397288317618
C	-0.12046356242524	1.76087564632878	-0.64811825724178
C	-0.72261481570134	1.56853594023263	-1.75961227097054
C	-1.95913018615634	2.04076883979766	-2.45236501573574
C	-1.81411010480347	2.80179191150875	-3.75437545404413
C	-0.86882650556278	3.81656876115746	-3.92208037762225
C	-0.75546050847793	4.49712418916634	-5.13575851460124
C	-1.59326994609443	4.20067127455830	-6.20220244664627
C	-2.56021199096439	3.20851958093212	-6.04071925643539
C	-2.66298971676126	2.52070047824131	-4.83333890593644
F	-0.03768995313334	4.15885108042491	-2.91505095975741
F	0.19112508347865	5.45452516357774	-5.25935612979151
N	-1.35402769278936	0.07724370830747	-6.71209280711335
N	-0.27671771258421	1.67405628553764	-8.73351968994071
H	0.96440928267383	2.36751185855453	1.78772785440681
H	2.95896809708702	1.29569973607397	2.78582717166407
H	4.15921314612775	-0.51019104079863	1.55066520951049
H	3.35472200464149	-1.23870749330660	-0.67313537586249
H	-0.15510083358744	-1.06905295137195	-4.32803719022874
H	-1.39808876586474	0.15647544598007	-4.14370269310584
H	-2.47867944099243	2.67759914652747	-1.72109538955393
H	-2.62604032840310	1.18557353966836	-2.63923029638741
H	1.82380816572519	3.14955536178047	-7.92887979229182
H	2.79446565060708	3.18659428228236	-5.63594439064679
H	1.84577696314482	1.70402368253766	-3.86723327381164
H	-3.39732212006345	1.72163165935584	-4.72778443188705
H	-3.21116524545369	2.94939995674268	-6.87388328959569
H	-1.46574159750820	4.73572591451111	-7.14148482877371
H	-1.70516119887021	0.14155243536976	-7.66097471275932
H	-1.36176782724341	-0.87056376196323	-6.35089540390541
H	0.20563905113797	2.29496626672067	-9.38036317826922
H	-0.31516948401324	0.74302251223222	-9.15311453902535

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Intermediate

C	1.41923349582913	1.73527945988996	-4.89154945881601
C	0.33517230938583	0.88972654545371	-5.14707063897581
C	-0.20686808318254	0.82750642954718	-6.44606379419137
C	0.34604764203143	1.62430773746779	-7.47509589000951
C	1.41511829711038	2.47651518718651	-7.18739767180629
C	1.95115892934708	2.53613779116101	-5.90078660995061
C	-0.31512821678023	0.04851951769783	-4.06422142047512
C	0.09311734654963	0.41542567143490	-2.65714252953428
C	1.18112435866563	-0.11881564689060	-2.05196710437273
C	1.69444411320847	0.16902095180794	-0.79264844277294
C	0.94506307159301	1.17664622631077	-0.01931717979484
C	1.41936977774044	1.52254798912324	1.27191321233169

C	2.55442020365679	0.93696203473217	1.79437644279146
C	3.27394448635228	-0.02750026619367	1.05205398695257
C	2.85398182551493	-0.40178728855814	-0.20804324932533
C	-0.17619240418654	1.70223019793725	-0.65039723185089
C	-0.65832903207363	1.41479468494459	-1.88280565008086
C	-1.93396000510001	2.04859604894145	-2.41627256050302
C	-1.81548956228887	2.81792840968979	-3.71268377997456
C	-0.86757571380049	3.83138545278278	-3.87128291436933
C	-0.73552168470486	4.51231633607274	-5.08174261578191
C	-1.55704001464467	4.21210955361970	-6.16018781449843
C	-2.52670850263363	3.22058291390607	-6.01051951864632
C	-2.64985100424983	2.53640077656515	-4.80257109431191
F	-0.04512416081035	4.16271151042123	-2.85016242811105
F	0.21432423761276	5.46837593243791	-5.19384869713040
N	-1.34285628802405	0.04636536688463	-6.70083157116498
N	-0.25620321516630	1.58417848351495	-8.76007710798950
H	0.86438279612085	2.26798317638731	1.84062711151947
H	2.90086096436329	1.22131124863671	2.78750385923103
H	4.17008757450139	-0.47740966909310	1.47856927071670
H	3.40877320249368	-1.14200763462893	-0.78370686270821
H	-0.06785611194371	-1.01540544808914	-4.22117430058758
H	-1.40746689532441	0.12814086601256	-4.17679833669391
H	-2.31675280261761	2.71047445297983	-1.62642703262123
H	-2.69169330107210	1.26349114707424	-2.56191679542959
H	1.83262069428466	3.09144884492677	-7.98715127914052
H	2.78149121706268	3.20744713263125	-5.68649439860670
H	1.82387411831949	1.78569957763833	-3.88188445521188
H	-3.38563071055716	1.73763787385858	-4.70566945479216
H	-3.16475067325876	2.95958652893464	-6.85310416983770
H	-1.41501081719015	4.74448779101842	-7.09890285785861
H	-1.68500905546237	0.07488966967396	-7.65447300202047
H	-1.35539099253696	-0.88528125532952	-6.30066811948652
H	0.23174804554297	2.18294877697370	-9.42336498139462
H	-0.29226545967759	0.63954191250554	-9.14825586271522