

Z,E-isomerism in series of substituted iminophosphonates: quantum chemical research

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Table S1. Calculated (M062X/6-311+G**) total energy values (E), zero point energy correction (ZPE), thermal correction to Gibbs free energy (TCGFE), corrected energy values (E+ZPE and E+TCGFE), relative energy values (ΔE and ΔG), lowest vibration frequency (ν , cm^{-1}) and valence angle at nitrogen (degree).

Structure	E, a.u.	$\nu(\text{cm}^{-1})$	ZPE, a.u.	E+ZPE, a.u.	ΔE , kcal/mol ^a	$\Delta E'$, kcal/mol ^b	TCGFE, a.u.	E+TCGFE, a.u.	ΔG , kJ/mol ^a	$\Delta G'$, kJ/mol ^b	ΔG^{exp} , kJ/mol	CNX angle, °
1-E	-1117.222366	30.7	0.157534	-1117.064832	0.00		0.113223	-1117.109143	0.00			122.8
1-Z	-1117.225013	15.5	0.157382	-1117.067631	-7.35		0.112536	-1117.112477	-8.75			122.0
1-TS	-1117.187865	-357.1	0.155534	-1117.032331	85.33	92.68	0.110333	-1117.077532	83.00	91.75		179.4
2-E	-1194.603835	29.3	0.192168	-1194.411667	0.00		0.145750	-1194.458085	0.00			123.5
2-Z	-1194.606636	15.8	0.192130	-1194.414506	-7.46		0.145486	-1194.461150	-8.05		-6.60	124.8
2-TS	-1194.572366	-232.8	0.190553	-1194.381813	78.38	85.84	0.144149	-1194.428217	78.42	86.47	81.90	178.3
3-E	-819.490432	38.5	0.179831	-819.310601	0.00		0.138662	-819.351770	0.00			118.1
3-Z	-819.488744	30.1	0.179956	-819.308788	4.76		0.138734	-819.350010	4.62			123.4
3-TS	-819.449264	-391.3	0.178025	-819.271239	103.35	98.59	0.136356	-819.312908	102.03	97.41		178.3
4-E	-1202.909120	16.2	0.286798	-1202.622322	0.00		0.236245	-1202.672875	-1.87			121.5
4-Z	-1202.911298	37.5	0.287125	-1202.624173	-4.86		0.239080	-1202.672218	1.73			123.3
4-TS	-1202.883872	-169.3	0.285275	-1202.598597	62.57	67.15	0.234665	-1202.649207	62.14	60.41		178.9
5-E	-1308.929851	27.7	0.210278	-1308.719573	6.03		0.161237	-1308.768614	6.17			124.3
5-Z	-1308.938594	35.4	0.210924	-1308.727670	-15.23		0.164126	-1308.774468	-9.20			122.6
5-TS	-1308.905822	-195.0	0.209007	-1308.696815	65.78	81.01	0.159351	-1308.746471	58.14	73.51	67.10	179.3
5'-E	-1308.932209	30.9	0.210338	-1308.721871	0.00		0.161245	-1308.770964	0.00			124.4
5'-Z	-1308.934293	25.7	0.210413	-1308.723880	-5.28		0.161986	-1308.772307	-3.53		-5.40	122.8
5'-TS	-1308.906386	-182.1	0.208975	-1308.697411	64.22	69.50	0.159857	-1308.746529	64.15	67.68		177.0
6-E	-1401.167848	28.8	0.208978	-1400.958870	0.00		0.157615	-1401.010233	0.00			124.0
6-Z	-1401.176916	41.9	0.209460	-1400.967456	-22.54		0.159958	-1401.016958	-17.66			122.2
6-TS	-1401.146145	-174.1	0.207716	-1400.938429	53.67	76.21	0.155189	-1400.990956	50.61	68.27	64.60	178.8

Table S1 (continued).

Structure	E, a.u.	$\nu(\text{cm}^{-1})$	ZPE, a.u.	E+ZPE, a.u.	ΔE , kcal/mol ^a	$\Delta E'$, kcal/mol ^b	TCGFE, a.u.	E+TCGFE, a.u.	ΔG , kJ/mol ^a	$\Delta G'$, kJ/mol ^b	ΔG^{exp} , kJ/mol	CNX angle, °
7-E	-1423.445109	24.6	0.243489	-1423.201620	0.00		0.191492	-1423.253617	0.00			126.2
7-Z	-1423.451752	42.6	0.243874	-1423.207878	-16.43		0.193954	-1423.257798	-10.98			122.0
7-TS	-1423.422303	-165.3	0.241986	-1423.180317	55.93	72.36	0.189813	-1423.232490	55.47	66.45	73.40	176.7
8-E	-1077.926113	33.5	0.129853	-1077.796260	0.00		0.087551	-1077.838562	0.00			111.8
8-Z	-1077.928907	32.6	0.129842	-1077.799065	-7.36		0.087513	-1077.841394	-7.43			109.9
8-TS	-1077.884982	-1076.2	0.127098	-1077.757884	100.76	102.01	0.084400	-1077.800582	99.72	107.15		178.4
9-E	-971.898362	27.3	0.206237	-971.692125	0.00		0.162892	-971.735470	0.00			110.9
9-Z	-971.905772	15.0	0.206369	-971.699403	-19.11		0.162068	-971.743704	-21.62			110.7
9-TS	-971.857421	-1116.4	0.203384	-971.654037	100.00	119.11	0.159306	-971.698115	119.69	98.07		177.3
10-E	-1486.575383	18.0	0.230943	-1486.344440	0.00		0.178973	-1486.396410	0.00			136.2
10-Z	-1486.582232	23.6	0.231065	-1486.351167	-17.66		0.179694	-1486.402538	-16.09			133.9
10-TS	-1486.570108	-66.3	0.230165	-1486.339943	11.81	29.47	0.177435	-1486.392673	9.81	25.90		176.5
11-E	-659.516068	43.0	0.090732	-659.425336	0.00		0.054659	-659.461409	0.00			109.9
11-Z	-659.502198	32.3	0.090544	-659.411654	35.92		0.054261	-659.447937	35.37			111.1
11-TS	-659.474678	-1069.6	0.088190	-659.386488	101.99	66.07	0.051835	-659.422843	101.25	65.88		179.7
12-E	-1068.169115	13.5	0.191871	-1067.977244	0.00		0.145302	-1068.023813	0.00			134.4
12-Z	-1068.163874	20.7	0.191758	-1067.972116	13.47		0.145160	-1068.018714	13.39			137.5
12-TS	-1068.158721	-67.2	0.191184	-1067.967537	25.49	12.02	0.144145	-1068.014576	24.25	10.86		179.4

^a Energy values calculated relative to E-isomer. ^b Energy values calculated relative to Z-isomer.

Table S2. Calculated (RI-MP2/cc-pVTZ//M062X/6-311+G**) total energy values (E(MP2)), zero point energy correction (ZPE, M062X/6-311+G**), thermal correction to Gibbs free energy (TCGFE, M062X/6-311+G**), corrected energy values (E+ZPE and E+TCGFE, without scaling) and relative energy values (ΔE and ΔG).

Structure	E(MP2), a.u.	ΔE , kcal/mol ^a	$\Delta E'$, kcal/mol ^b	ZPE, a.u.	E+ZPE, a.u.	ΔG , kJ/mol ^a	$\Delta G'$, kJ/mol ^b
5-E	-1306.907032			0.161237	-1306.745795		19.14
5'-E	-1306.914332			0.161245	-1306.753087	0.00	
5'-Z	-1306.915601			0.161986	-1306.753615	-1.39 ^c	
5-Z	-1306.918473			0.164126	-1306.754347	-3.31 ^e	
5'-TS	-1306.883271	81.55	84.88	0.159857	-1306.723414	77.90 ^c	79.29 ^d
5-TS	-1306.884837	58.27	88.31	0.159351	-1306.725486	53.32 ^e	75.77 ^f
6-E	-1398.981294			0.157615	-1398.823679	0.00	
6-Z	-1398.988589			0.159958	-1398.828631	-13.00	
6-TS	-1398.955950	66.54	85.69	0.155189	-1398.800761	60.17	73.17
7-E	-1421.235817			0.191492	-1421.044325	0.00	
7-Z	-1421.240309			0.193954	-1421.046355	-5.33	
7-TS	-1421.207267	74.96	86.75	0.189813	-1421.017454	70.55	75.88

^a Energy values calculated relative to E-isomer. ^b Energy values calculated relative to Z-isomer. ^c Relative to 5'-E. ^d Relative to 5'-Z. ^e Relative to 5-E.

^f Relative to 5-Z.

Table S3. Calculated (M062X/6-311+G**) total energy values with taking into account solvent effects (PCM and CPCM methods), zero point energy correction (ZPE, M062X/6-311+G**), and corrected energy values (E+ZPE, without scaling), relative energy values (ΔE).

Structure	Solvent model	toluene				methanol				chloroform			
		E, a.u.	ZPE, a.u.	E+ZPE, a.u.	ΔE^* , kJ/mol ^a	E, a.u.	ZPE, a.u.	E+ZPE, a.u.	ΔE^* , kJ/mol ^a	E, a.u.	ZPE, a.u.	E+ZPE, a.u.	ΔE^* , kJ/mol ^a
1-E	PCM	-1117.227768	0.157534	-1117.070234	0.0	-1117.233526	0.157534	-1117.075992	0.0	-1117.230538	0.157534	-1117.073004	0.0
	CPCM	-1117.228773	0.157534	-1117.071239	0.0	-1117.233692	0.157534	-1117.076158	0.0	-1117.231340	0.157534	-1117.073806	0.0
1-Z	PCM	-1117.230178	0.157382	-1117.072796	-6.7	-1117.235707	0.157382	-1117.078325	-6.1	-1117.232840	0.157382	-1117.075458	-6.4
	CPCM	-1117.231188	0.157382	-1117.073806	-6.7	-1117.235874	0.157382	-1117.078492	-6.1	-1117.233644	0.157382	-1117.076262	-6.4
1-TS	PCM	-1117.193820	0.155534	-1117.038286	90.6	-1117.199937	0.155534	-1117.044403	89.1	-1117.196773	0.155534	-1117.041239	89.8
	CPCM	-1117.194863	0.155534	-1117.039329	90.5	-1117.200113	0.155534	-1117.044579	89.0	-1117.197611	0.155534	-1117.042077	89.8
2-E	PCM	-1194.609528	0.192168	-1194.417360	0.0	-1194.615699	0.192168	-1194.423531	0.0	-1194.612483	0.192168	-1194.420315	0.0
	CPCM	-1194.610625	0.192168	-1194.418457	0.0	-1194.615883	0.192168	-1194.423715	0.0	-1194.613364	0.192168	-1194.421196	0.0
2-Z	PCM	-1194.610625	0.192168	-1194.418457	0.0	-1194.615883	0.192168	-1194.423715	0.0	-1194.613364	0.192168	-1194.421196	0.0
	CPCM	-1194.611730	0.192130	-1194.419600	-5.9	-1194.617225	0.192130	-1194.425095	-4.1	-1194.614360	0.192130	-1194.422230	-5.0
2-TS	PCM	-1194.574715	0.190553	-1194.384162	75.6	-1194.581474	0.190553	-1194.390921	73.1	-1194.577910	0.190553	-1194.387357	74.5
	CPCM	-1194.575954	0.190553	-1194.385401	75.3	-1194.581694	0.190553	-1194.391141	73.0	-1194.578931	0.190553	-1194.388378	74.2
3-E	PCM	-819.496397	0.179831	-819.316566	0.0	-819.5027856	0.179831	-819.322955	0.0	-819.499463	0.179831	-819.319632	0.0
	CPCM	-819.497504	0.179831	-819.317673	0.0	-819.5029703	0.179831	-819.323139	0.0	-819.500350	0.179831	-819.320519	0.0
3-Z	PCM	-819.491362	0.179956	-819.311406	13.5	-819.4964601	0.179956	-819.316504	16.9	-819.493785	0.179956	-819.313829	15.2
	CPCM	-819.492385	0.179956	-819.312429	13.8	-819.4966329	0.179956	-819.316677	17.0	-819.494607	0.179956	-819.314651	15.4
3-TS	PCM	-819.454656	0.178025	-819.276631	91.3	-819.4605502	0.178025	-819.282525	89.2	-819.457464	0.178025	-819.279439	90.3
	CPCM	-819.455718	0.178025	-819.277693	91.2	-819.4607344	0.178025	-819.282709	89.2	-819.458329	0.178025	-819.280304	90.2
4-E	PCM	-1202.916083	0.286798	-1202.629285	0.0	-1202.923897	0.286798	-1202.637099	0.0	-1202.919737	0.286798	-1202.632939	0.0
	CPCM	-1202.917725	0.286798	-1202.630927	0.0	-1202.924185	0.286798	-1202.637387	0.0	-1202.921083	0.286798	-1202.634285	0.0
4-Z	PCM	-1202.917132	0.287125	-1202.630007	-1.9	-1202.923996	0.287125	-1202.636871	0.6	-1202.920325	0.287125	-1202.633200	-0.7
	CPCM	-1202.918642	0.287125	-1202.631517	-1.5	-1202.924263	0.287125	-1202.637138	0.7	-1202.921568	0.287125	-1202.634443	-0.4
4-TS	PCM	-1202.888536	0.285275	-1202.603261	70.2	-1202.895473	0.285275	-1202.610198	70.0	-1202.891806	0.285275	-1202.606531	70.0
	CPCM	-1202.889997	0.285275	-1202.604722	70.3	-1202.895725	0.285275	-1202.610450	70.1	-1202.892993	0.285275	-1202.607718	70.2

Table S3 (continued).

Structure	Solvent model	toluene				methanol				chloroform			
		E, a.u.	ZPE, a.u.	E+ZPE, a.u.	ΔE^* , kJ/mol ^a	E, a.u.	ZPE, a.u.	E+ZPE, a.u.	ΔE^* , kJ/mol ^a	E, a.u.	ZPE, a.u.	E+ZPE, a.u.	ΔE^* , kJ/mol ^a
5-E	PCM	-1308.937982	0.210278	-1308.727704	0.0	-1308.944367	0.210278	-1308.734089	0.0	-1308.941030	0.210278	-1308.730752	0.0
	CPCM	-1308.939204	0.210278	-1308.728926	0.0	-1308.944573	0.210278	-1308.734295	0.0	-1308.942012	0.210278	-1308.731734	0.0
5-Z	PCM	-1308.944136	0.210338	-1308.733798	-16.0	-1308.950256	0.210338	-1308.739918	-15.3	-1308.947046	0.210338	-1308.736708	-15.6
	CPCM	-1308.945304	0.210338	-1308.734966	-15.9	-1308.950457	0.210338	-1308.740119	-15.3	-1308.947046	0.210338	-1308.736708	-13.1
5-TS	PCM	-1308.911842	0.210413	-1308.701429	85.0	-1308.918208	0.210413	-1308.707795	84.3	-1308.914884	0.210413	-1308.704471	84.6
	CPCM	-1308.913052	0.210413	-1308.702639	84.9	-1308.918412	0.210413	-1308.707999	84.3	-1308.915857	0.210413	-1308.705444	82.1
5'-E	PCM	-1308.935898	0.210924	-1308.724974	0.0	-1308.942721	0.210924	-1308.731797	0.0	-1308.939119	0.210924	-1308.728195	0.0
	CPCM	-1308.937298	0.210924	-1308.726374	0.0	-1308.942964	0.210924	-1308.732040	0.0	-1308.940259	0.210924	-1308.729335	0.0
5'-Z	PCM	-1308.940422	0.208975	-1308.731447	-17.0	-1308.947666	0.208975	-1308.738690	-18.1	-1308.943760	0.208975	-1308.734784	-17.3
	CPCM	-1308.942084	0.208975	-1308.733109	-17.7	-1308.947980	0.208975	-1308.739004	-18.3	-1308.945162	0.208975	-1308.736187	-18.0
5'-TS	PCM	-1308.911884	0.209007	-1308.702877	75.0	-1308.917871	0.209007	-1308.708864	78.3	-1308.914733	0.209007	-1308.705726	76.3
	CPCM	-1308.913040	0.209007	-1308.704033	76.3	-1308.918068	0.209007	-1308.709061	78.6	-1308.915667	0.209007	-1308.706660	77.5
6-E	PCM	-1401.176150	0.208978	-1400.967172	0.0	-1401.185150	0.208978	-1400.976172	0.0	-1401.180454	0.208978	-1400.971476	0.0
	CPCM	-1401.177753	0.208978	-1400.968775	0.0	-1401.185423	0.208978	-1400.976445	0.0	-1401.181750	0.208978	-1400.972772	0.0
6-Z	PCM	-1401.184142	0.209460	-1400.974682	-19.7	-1401.191791	0.209460	-1400.982331	-16.2	-1401.187826	0.209460	-1400.978366	-18.1
	CPCM	-1401.185468	0.209460	-1400.976008	-19.0	-1401.192011	0.209460	-1400.982551	-16.0	-1401.188885	0.209460	-1400.979425	-17.5
6-TS	PCM	-1401.154808	0.207716	-1400.947092	72.4	-1401.163854	0.207716	-1400.956138	68.8	-1401.159168	0.207716	-1400.951452	70.7
	CPCM	-1401.156242	0.207716	-1400.948526	72.2	-1401.164098	0.207716	-1400.956382	68.7	-1401.160324	0.207716	-1400.952608	70.4
7-E	PCM	-1423.451939	0.243489	-1423.208450	0.0	-1423.459423	0.243489	-1423.215934	0.0	-1423.455512	0.243489	-1423.212023	0.0
	CPCM	-1423.453330	0.243489	-1423.209841	0.0	-1423.459656	0.243489	-1423.216167	0.0	-1423.456631	0.243489	-1423.213142	0.0
7-Z	PCM	-1423.457800	0.243874	-1423.213926	-14.4	-1423.464364	0.243874	-1423.220490	-12.0	-1423.460926	0.243874	-1423.217052	-13.2
	CPCM	-1423.459090	0.243874	-1423.215216	-14.1	-1423.464581	0.243874	-1423.220707	-11.9	-1423.461964	0.243874	-1423.218090	-13.0
7-TS	PCM	-1423.428933	0.241986	-1423.186947	70.8	-1423.435991	0.241986	-1423.194005	69.5	-1423.432312	0.241986	-1423.190326	70.2
	CPCM	-1423.430223	0.241986	-1423.188237	70.8	-1423.436208	0.241986	-1423.194222	69.5	-1423.433350	0.241986	-1423.191364	70.2
8-E	PCM	-1077.931558	0.129853	-1077.801705	0.0	-1077.937432	0.129853	-1077.807579	0.0	-1077.934364	0.129853	-1077.804511	0.0
	CPCM	-1077.932672	0.129853	-1077.802819	0.0	-1077.937619	0.129853	-1077.807766	0.0	-1077.935259	0.129853	-1077.805406	0.0
8-Z	PCM	-1077.934254	0.129842	-1077.804412	-7.1	-1077.939877	0.129842	-1077.810035	-6.4	-1077.936958	0.129842	-1077.807116	-6.8
	CPCM	-1077.935325	0.129842	-1077.805483	-7.0	-1077.940056	0.129842	-1077.810214	-6.4	-1077.937814	0.129842	-1077.807972	-6.7

Table S3 (continued).

Structure	Solvent model	toluene				methanol				chloroform			
		E, a.u.	ZPE, a.u.	E+ZPE, a.u.	ΔE^* , kJ/mol ^a	E, a.u.	ZPE, a.u.	E+ZPE, a.u.	ΔE^* , kJ/mol ^a	E, a.u.	ZPE, a.u.	E+ZPE, a.u.	ΔE^* , kJ/mol ^a
8-TS	PCM	-1077.888879	0.127098	-1077.761781	111.9	-1077.895352	0.127098	-1077.768254	109.7	-1077.892004	0.127098	-1077.764906	110.8
	CPCM	-1077.890022	0.127098	-1077.762924	111.7	-1077.895539	0.127098	-1077.768441	109.7	-1077.892910	0.127098	-1077.765812	110.7
9-E	PCM	-971.905622	0.206237	-971.699385	0.0	-971.914103	0.206237	-971.707866	0.0	-971.909595	0.206237	-971.703358	0.0
	CPCM	-971.907285	0.206237	-971.701048	0.0	-971.914400	0.206237	-971.708163	0.0	-971.910969	0.206237	-971.704732	0.0
9-Z	PCM	-971.911386	0.206467	-971.704919	-14.5	-971.917473	0.206467	-971.711006	-8.2	-971.914293	0.206467	-971.707826	-11.7
	CPCM	-971.912540	0.206467	-971.706073	-13.2	-971.917665	0.206467	-971.711198	-8.0	-971.915217	0.206467	-971.708750	-10.5
9-TS	PCM	-971.864623	0.203384	-971.661239	114.7	-971.872955	0.203384	-971.669571	108.8	-971.868543	0.203384	-971.665159	112.0
	CPCM	-971.866212	0.203384	-971.662828	113.5	-971.873232	0.203384	-971.669848	108.6	-971.869843	0.203384	-971.666459	111.0
10-E	PCM	-1486.581050	0.230943	-1486.350107	0.0	-1486.587492	0.230943	-1486.356549	0.0	-1486.584071	0.230943	-1486.353128	0.0
	CPCM	-1486.582390	0.230943	-1486.351447	0.0	-1486.587732	0.230943	-1486.356789	0.0	-1486.585176	0.230943	-1486.354233	0.0
10-Z	PCM	-1486.586663	0.231065	-1486.355598	-14.4	-1486.591795	0.231065	-1486.360730	-11.0	-1486.589066	0.231065	-1486.358001	-12.8
	CPCM	-1486.587795	0.231065	-1486.356730	-13.9	-1486.591996	0.231065	-1486.360931	-10.9	-1486.589997	0.231065	-1486.358932	-12.3
10-TS	PCM	-1486.575644	0.230165	-1486.345479	26.6	-1486.581901	0.230165	-1486.351736	23.6	-1486.578571	0.230165	-1486.348406	25.2
	CPCM	-1486.576917	0.230165	-1486.346752	26.2	-1486.582142	0.230165	-1486.351977	23.5	-1486.579643	0.230165	-1486.349478	24.8
11-E	PCM	-659.520468	0.090732	-659.429736	0.0	-659.525417	0.090732	-659.434685	0.0	-659.522805	0.090732	-659.432073	0.0
	CPCM	-659.521448	0.090732	-659.430716	0.0	-659.525589	0.090732	-659.434857	0.0	-659.523607	0.090732	-659.432875	0.0
11-Z	PCM	-659.518473	0.090544	-659.427929	4.7	-659.523482	0.090544	-659.432938	4.6	-659.520806	0.090544	-659.430262	4.8
	CPCM	-659.519642	0.090544	-659.429098	4.2	-659.523687	0.090544	-659.433143	4.5	-659.521764	0.090544	-659.431220	4.3
11-TS	PCM	-659.479422	0.088190	-659.391232	96.3	-659.484537	0.088190	-659.396347	96.1	-659.481868	0.088190	-659.393678	96.1
	CPCM	-659.480388	0.088190	-659.392198	96.9	-659.484699	0.088190	-659.396509	96.2	-659.482644	0.088190	-659.394454	96.5
12-E	PCM	-1068.172480	0.191871	-1067.980609	0.0	-1068.176286	0.191871	-1067.984415	0.0	-1068.174268	0.191871	-1067.982397	0.0
	CPCM	-1068.173311	0.191871	-1067.981440	0.0	-1068.176434	0.191871	-1067.984563	0.0	-1068.174953	0.191871	-1067.983082	0.0
12-Z	PCM	-1068.167911	0.191758	-1067.976153	11.7	-1068.172614	0.191758	-1067.980856	9.3	-1068.170093	0.191758	-1067.978335	10.7
	CPCM	-1068.168952	0.191758	-1067.977194	11.1	-1068.172806	0.191758	-1067.981048	9.2	-1068.170964	0.191758	-1067.979206	10.2
12-TS	PCM	-1068.162285	0.191184	-1067.971101	13.3	-1068.166338	0.191184	-1067.975154	15.0	-1068.164181	0.191184	-1067.972997	14.0
	CPCM	-1068.163149	0.191184	-1067.971965	13.7	-1068.166499	0.191184	-1067.975315	15.1	-1068.164906	0.191184	-1067.973722	14.4

* ΔE values are given relative to the energy of E-isomer.

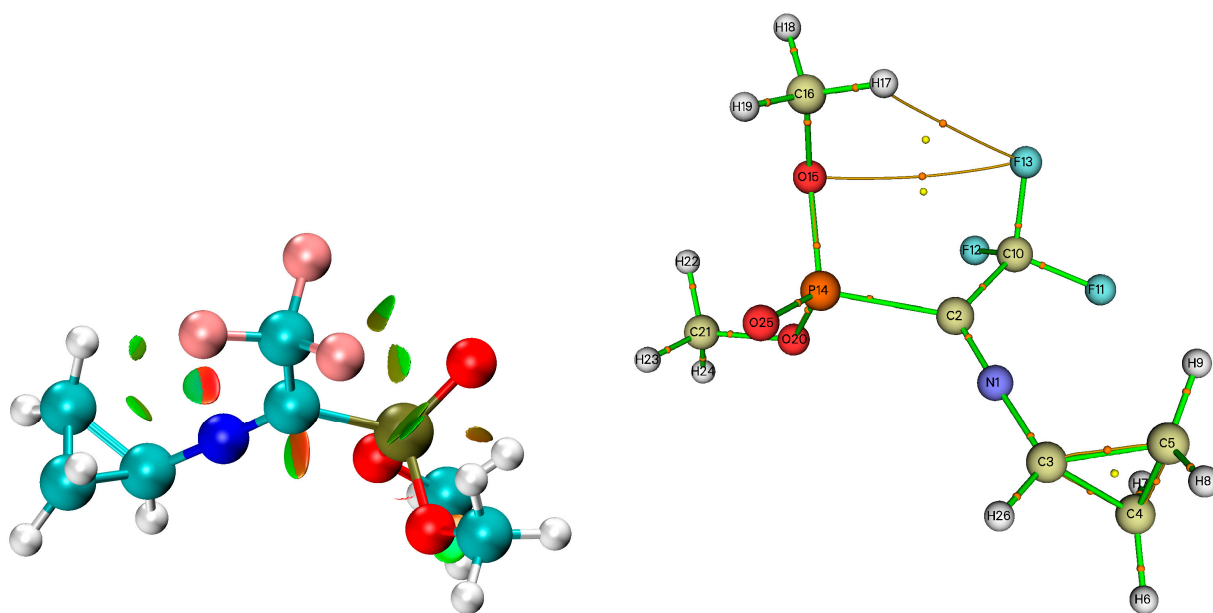
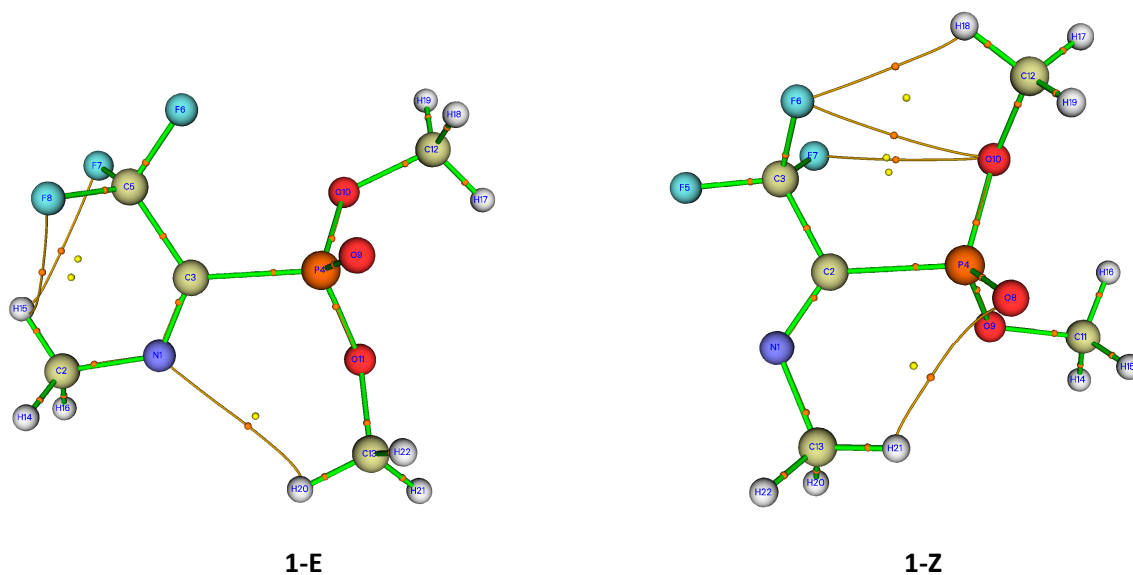
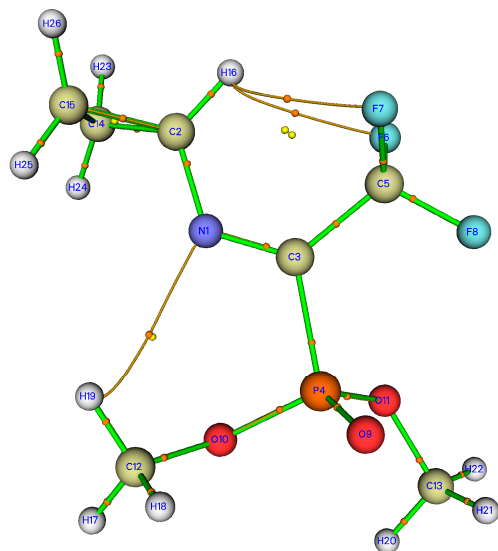
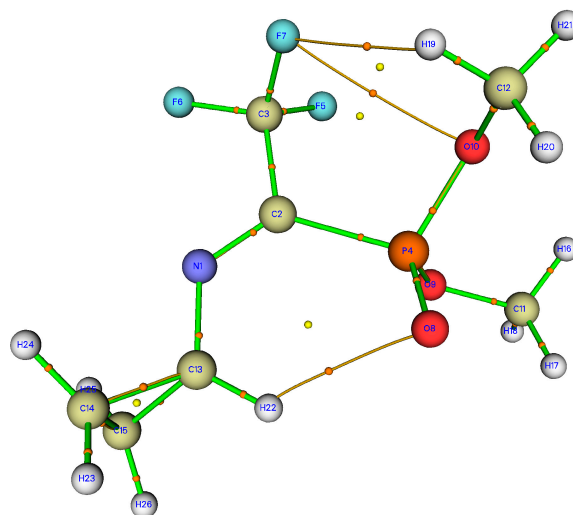


Figure S1. An illustration of weak C-F ...H-C attraction (green) (left) and bond critical points of type (3, -1) and (3, +1) (CPs) (right) for **2-TS** structure.

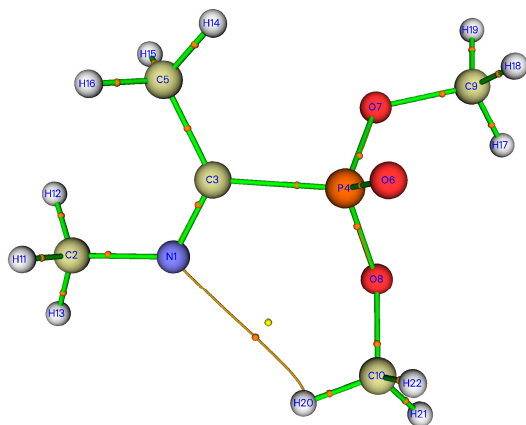




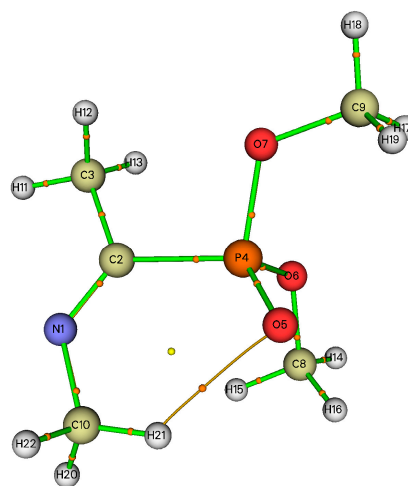
2-E



2-Z

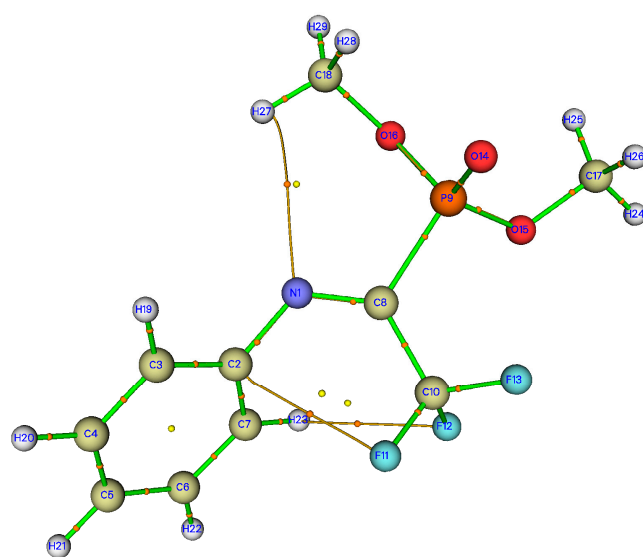


3-E

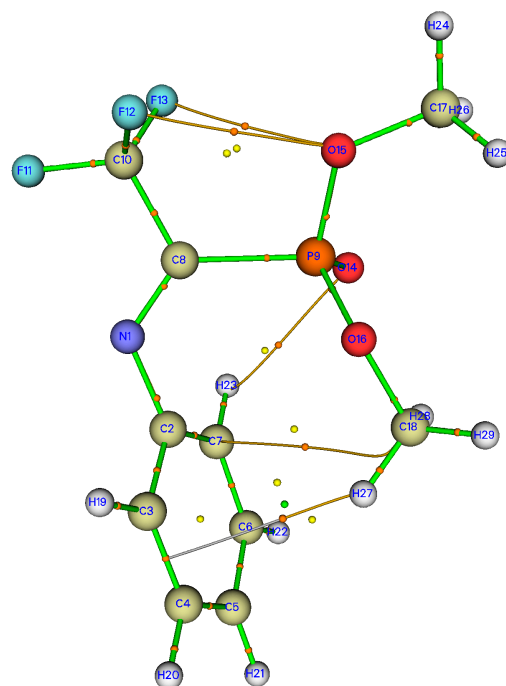


3-Z

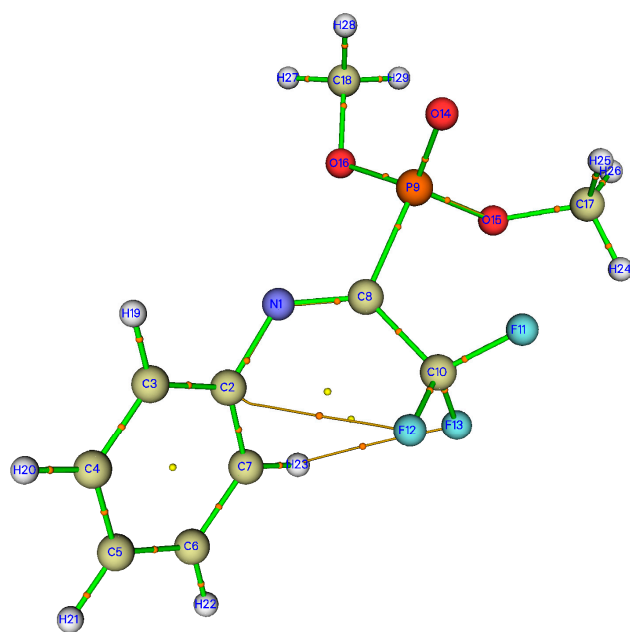
Figure S2. Bond critical points of type (3, -1) and (3, +1) (CPs) for E- and Z-isomers of **1-7**.



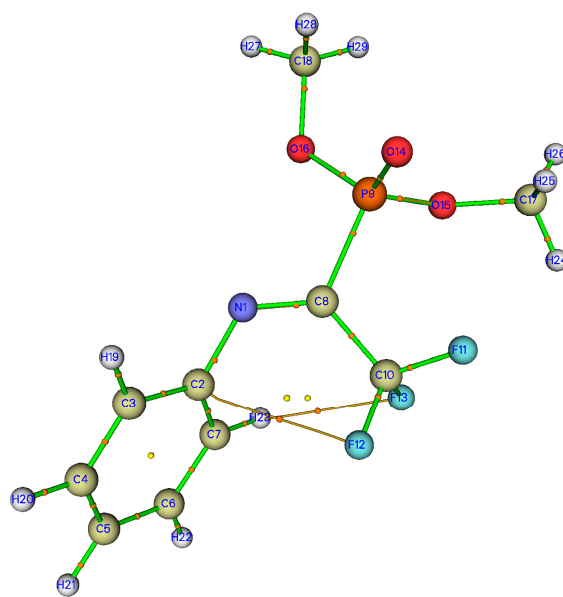
5-E



5-Z

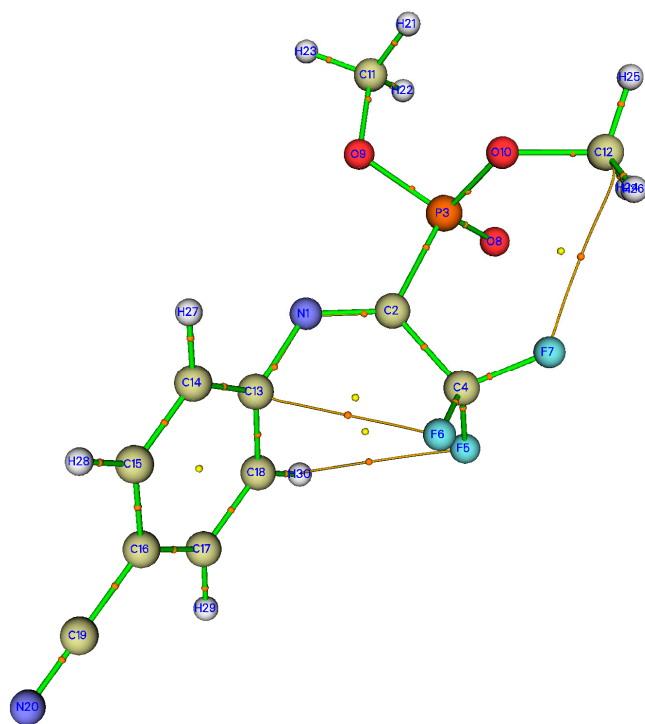


5'-E

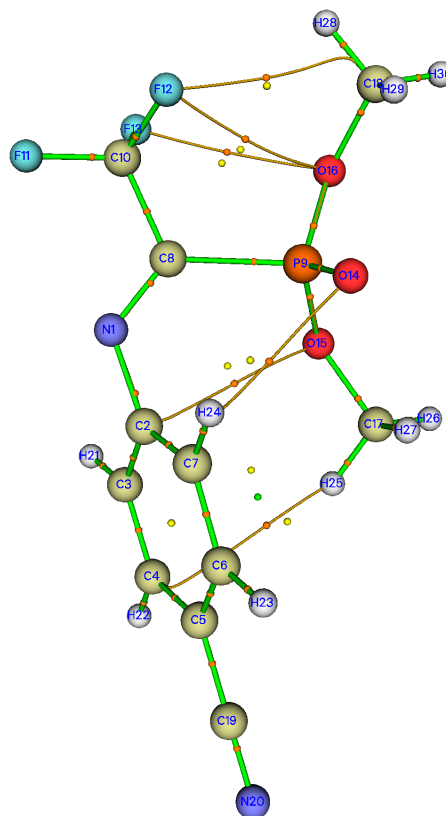


5'-Z

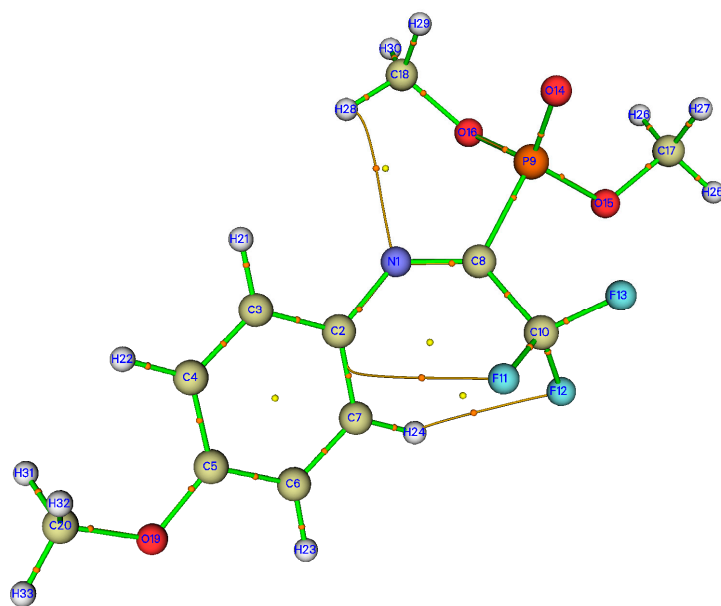
Figure S2 (continued). Bond critical points of type (3, -1) and (3, +1) (CPs) for E- and Z-isomers of **1-7**.



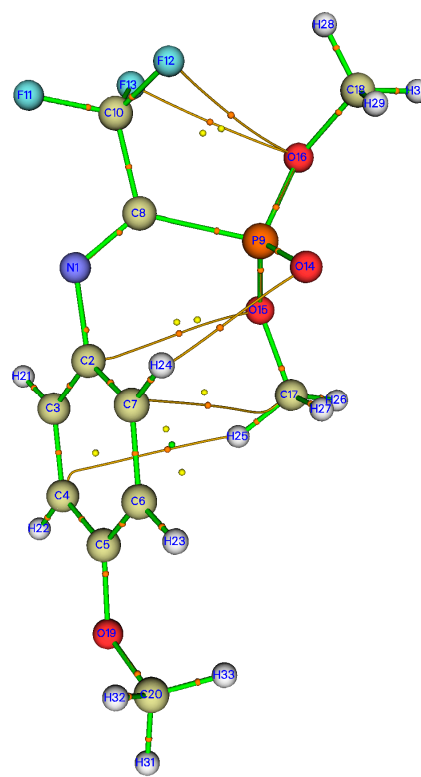
6-E



6-Z



7-E



7-Z

Figure S2 (continued). Bond critical points of type (3, -1) and (3, +1) (CPs) for E- and Z-isomers of **1-7**.

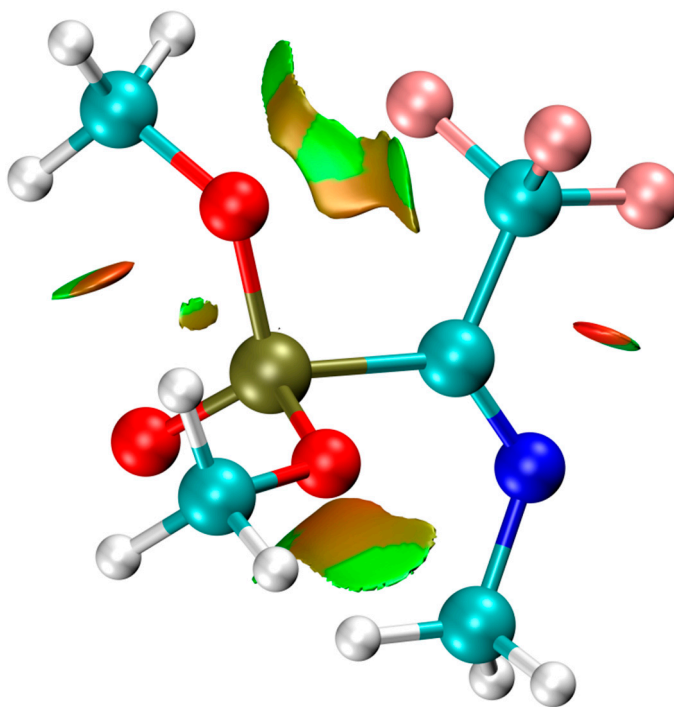
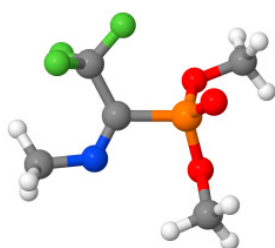


Figure S3. An illustration of non-covalent interactions for compound **1-Z**. Gradient isosurfaces ($s=0.5$ a.u.) are colored on a blue-green-red scale according to the character of interaction, where blue indicates attractive interactions and red indicates strong repulsive interactions.

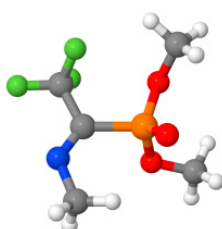
Cartesian coordinates for equilibrium (M062X/6-311+G**) structures

1-E



N	0.92296	1.58911	-0.37930
C	2.28251	2.07011	-0.56675
C	0.65725	0.39489	-0.08185
P	-1.10512	-0.02400	0.20617
C	1.70178	-0.70353	0.13884
F	1.14246	-1.82559	0.58332
F	2.34706	-0.98911	-1.00030
F	2.62098	-0.32599	1.03656
O	-1.43485	-0.27962	1.61832
O	-1.30223	-1.21903	-0.82116
O	-1.92803	1.15346	-0.47778
C	-2.46749	-2.05205	-0.71867
C	-2.21981	2.35607	0.24998
H	2.53364	2.68178	0.30329
H	3.03973	1.29572	-0.69303
H	2.27869	2.72715	-1.43648
H	-3.35861	-1.47696	-0.97571
H	-2.55313	-2.45117	0.29254
H	-2.32738	-2.85810	-1.43374
H	-1.34731	3.00878	0.22554
H	-3.05697	2.82727	-0.25954
H	-2.49171	2.11663	1.27908

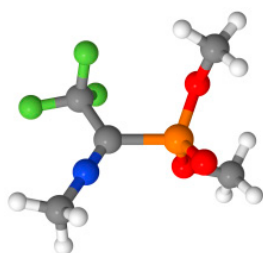
1-Z



N	-1.05891	1.90552	-0.26592
C	-0.74897	0.69977	-0.10156
C	-1.86639	-0.26775	0.26729
P	0.94317	-0.01823	-0.28036
F	-3.06081	0.29944	0.25678
F	-1.89020	-1.29170	-0.60911
F	-1.66481	-0.79109	1.48180
O	1.56326	0.17553	-1.60236
O	1.64587	0.68935	0.96098
O	0.84324	-1.53703	0.19190

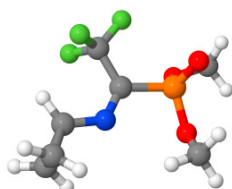
C	3.01615	0.37508	1.25589
C	0.87743	-2.63008	-0.74307
C	-0.07340	2.91298	-0.60993
H	3.31668	1.04388	2.05764
H	3.63817	0.54111	0.37491
H	3.09276	-0.66177	1.58654
H	1.36393	-3.45668	-0.23083
H	-0.14271	-2.90198	-1.00904
H	1.44081	-2.34754	-1.63240
H	0.05231	3.55045	0.26826
H	0.89563	2.52354	-0.92826
H	-0.49813	3.53129	-1.40110

1-TS



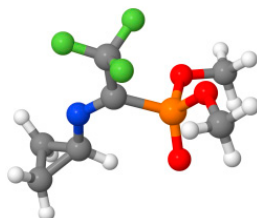
N	1.49663	1.42716	-0.26329
C	2.26557	2.57201	-0.53892
C	0.83806	0.42257	-0.02412
P	-1.01253	0.43197	-0.19384
C	1.49404	-0.91433	0.38359
F	0.88283	-1.46365	1.43540
F	1.42197	-1.79553	-0.63026
F	2.77950	-0.75147	0.68457
O	-1.50298	1.44892	-1.13833
O	-1.46296	0.55292	1.32740
O	-1.45665	-1.07220	-0.53761
C	-2.86121	0.53134	1.65158
C	-1.53075	-1.48986	-1.90750
H	2.12967	3.25910	0.30080
H	3.33356	2.35822	-0.64566
H	1.88534	3.07999	-1.42943
H	-2.93023	0.72791	2.71809
H	-3.27667	-0.45140	1.42448
H	-3.38855	1.30612	1.09276
H	-0.52631	-1.57839	-2.32652
H	-2.00959	-2.46577	-1.90384
H	-2.11798	-0.77707	-2.48696

2-E



N	1.22900	0.63865	-0.13495
C	2.60387	0.31192	-0.21380
C	0.31678	-0.21965	0.03792
P	-1.39805	0.39219	0.19448
C	0.56618	-1.71687	0.20131
F	1.15250	-2.22931	-0.89009
F	1.37514	-1.96733	1.23991
F	-0.56827	-2.38233	0.40342
O	-1.98465	0.21389	1.53373
O	-1.34491	1.89958	-0.31911
O	-2.10539	-0.35742	-1.01422
C	-1.00979	2.95827	0.58848
C	-3.53938	-0.38894	-1.07944
C	3.40306	1.20759	-1.13491
C	3.53111	1.37209	0.33881
H	2.91634	-0.72135	-0.12514
H	-1.37398	3.87783	0.13657
H	-1.49261	2.79580	1.55311
H	0.07345	3.00122	0.70591
H	-3.92242	0.60788	-1.30394
H	-3.94830	-0.74735	-0.13416
H	-3.79163	-1.07358	-1.88459
H	4.20827	0.73350	-1.67895
H	2.83479	1.94808	-1.67996
H	3.05269	2.22657	0.79664
H	4.42548	1.01380	0.82950

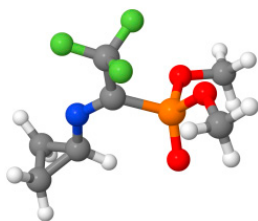
2-Z



N	-1.71018	0.38147	-0.02246
C	-0.45291	0.48542	-0.06746
C	0.11073	1.87374	-0.34117
P	0.77952	-0.85899	0.17273
F	1.02552	1.83569	-1.31752
F	-0.82468	2.74520	-0.68912
F	0.72461	2.35646	0.75704
O	0.36472	-1.91611	1.11186
O	1.04519	-1.27857	-1.33532
O	2.14631	-0.12951	0.56272
C	2.07146	-2.23949	-1.63040
C	2.49610	0.05869	1.94355
C	-2.39314	-0.82964	0.22181
C	-3.71919	-0.66070	0.93241
C	-3.70526	-0.95724	-0.52483
H	3.04901	-1.81508	-1.39868
H	1.90670	-3.15375	-1.05809

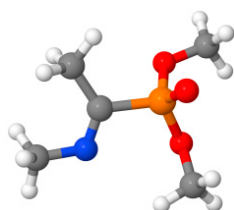
H	1.99633	-2.44642	-2.69430
H	1.88403	0.85151	2.37544
H	2.35675	-0.87092	2.49525
H	3.54127	0.35659	1.95225
H	-1.82401	-1.72849	0.42428
H	-3.98614	-1.44730	1.62451
H	-3.96550	0.34601	1.23943
H	-3.94198	-0.15217	-1.20611
H	-3.96369	-1.95271	-0.85873

2-TS



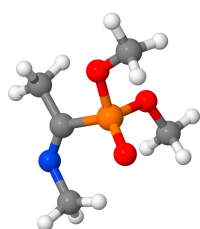
N	1.21134	0.72628	0.13769
C	0.38798	-0.17352	-0.06713
C	2.13858	1.69102	0.33712
C	3.40926	1.30843	1.09005
C	3.48105	1.48023	-0.37026
H	3.82154	2.08196	1.73413
H	3.42570	0.30003	1.49531
H	3.94106	2.37170	-0.78999
H	3.53220	0.58446	-0.98463
C	0.85596	-1.61564	-0.27977
F	2.14668	-1.73655	0.04317
F	0.16665	-2.49071	0.46400
F	0.71604	-1.97548	-1.55592
P	-1.41935	0.15073	-0.24180
O	-2.00936	0.37331	1.24459
C	-2.62681	-0.72726	1.90617
H	-2.16701	-1.68170	1.63370
H	-2.49198	-0.56221	2.97836
H	-3.69336	-0.76634	1.66090
O	-1.35482	1.67225	-0.73490
C	-2.59526	2.37162	-0.81058
H	-2.95619	2.60534	0.19733
H	-3.34293	1.77317	-1.34673
H	-2.40693	3.29762	-1.35857
O	-2.16424	-0.82850	-1.05775
H	1.80717	2.73006	0.43305

3-E



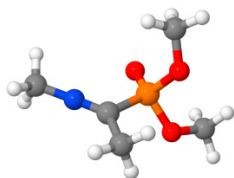
N	1.91119	0.49550	-0.30972
C	3.33716	0.22491	-0.43428
C	1.15254	-0.45208	0.05196
P	-0.60134	-0.01514	0.26748
C	1.55277	-1.86807	0.38614
O	-1.04344	0.02789	1.67580
O	-1.30044	-1.11914	-0.65315
O	-0.87645	1.32155	-0.55966
C	-2.73201	-1.17709	-0.69293
C	-0.61028	2.59932	0.03455
H	3.79470	0.17906	0.55965
H	3.54142	-0.71949	-0.94821
H	3.80524	1.03813	-0.98562
H	0.75216	-2.38451	0.91462
H	1.76224	-2.41887	-0.53552
H	2.45163	-1.87967	1.00554
H	-3.12421	-0.29429	-1.20059
H	-3.13412	-1.23872	0.31970
H	-2.98990	-2.07204	-1.25348
H	0.46082	2.79663	-0.00616
H	-1.15266	3.33310	-0.55735
H	-0.96400	2.61494	1.06670

3-Z



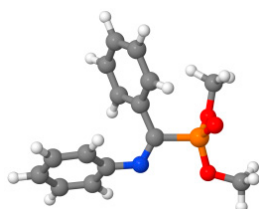
N	-2.49481	-0.01749	0.06572
C	-1.35814	-0.13771	0.60998
C	-1.26314	-0.45596	2.08331
P	0.28649	0.03495	-0.19535
O	0.43716	0.34755	-1.63387
O	0.95114	1.13995	0.77485
O	0.93805	-1.37657	0.23336
C	2.01502	1.95645	0.27401
C	2.06804	-1.86510	-0.49633
C	-2.67866	0.28805	-1.34323
H	-2.27428	-0.53109	2.48606
H	-0.72943	-1.39875	2.23708
H	-0.70931	0.32871	2.60786
H	2.05854	2.83760	0.91388
H	1.81947	2.24577	-0.76054
H	2.96405	1.41519	0.33343
H	2.97949	-1.35909	-0.16317
H	2.14403	-2.92960	-0.27529
H	1.92802	-1.70808	-1.56799
H	-3.28641	1.19612	-1.40389
H	-1.76056	0.41855	-1.92033
H	-3.27672	-0.51890	-1.77803

3-TS



N	-2.19714	-0.18077	-0.17040
C	-1.16680	-0.56007	0.38985
C	-1.05915	-1.46300	1.60548
P	0.45472	0.05234	-0.28340
O	0.40158	0.75558	-1.57858
O	1.11298	0.94912	0.89710
O	1.37558	-1.25543	-0.19430
C	0.86475	2.35721	0.90518
C	2.74649	-1.16649	-0.60200
C	-3.39239	0.22177	-0.78842
H	-2.05276	-1.66668	2.00310
H	-0.56994	-2.39838	1.32333
H	-0.43702	-0.99148	2.37080
H	1.51113	2.78301	1.66947
H	-0.17985	2.55868	1.15794
H	1.09301	2.78842	-0.07009
H	3.29660	-0.52222	0.08602
H	3.14709	-2.17652	-0.56649
H	2.81142	-0.77369	-1.61814
H	-3.54754	-0.43212	-1.65101
H	-4.27246	0.13733	-0.13896
H	-3.31894	1.24326	-1.17642

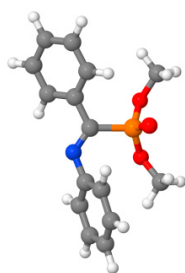
4-E



N	0.48988	-1.37833	-0.12157
C	-0.28768	-0.37716	-0.15886
P	-2.08793	-0.69122	-0.25384
C	0.06281	1.07390	-0.07172
O	-2.72763	-0.19094	-1.48877
O	-2.21738	-2.23776	0.05894
O	-2.68277	-0.02629	1.08363
C	-3.51267	-2.84722	-0.01399
C	-3.15091	1.32855	1.09601
C	1.89588	-1.22232	-0.10839
C	-0.46525	1.98372	-0.99130
C	-0.16889	3.33811	-0.87224
C	0.63270	3.79032	0.16984
C	2.56934	-0.46023	-1.06528
C	3.95628	-0.39041	-1.03906
C	4.67825	-1.06497	-0.05851

C	4.00463	-1.83451	0.88553
C	2.61934	-1.93276	0.84975
C	1.14765	2.88497	1.09557
C	0.86921	1.53046	0.97409
H	-4.16419	-2.43274	0.75785
H	-3.94956	-2.68752	-1.00093
H	-3.35869	-3.90871	0.16133
H	-3.91186	1.38888	1.87175
H	-3.57986	1.58986	0.12712
H	-2.32350	2.00059	1.33319
H	-1.10900	1.62774	-1.78824
H	-0.57046	4.03999	-1.59356
H	0.85531	4.84657	0.26469
H	2.00363	0.06413	-1.82660
H	4.47524	0.19529	-1.78862
H	5.75945	-1.00229	-0.03923
H	4.56008	-2.37465	1.64317
H	2.07940	-2.54932	1.55844
H	1.76891	3.23480	1.91129
H	1.27304	0.82107	1.68783

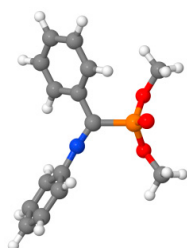
4-Z



N	0.39536	-1.42775	-0.04142
C	1.78173	-1.21762	0.07863
C	2.63961	-1.69455	-0.91542
C	4.01296	-1.56545	-0.76133
C	4.54554	-0.99858	0.39634
C	3.68962	-0.54657	1.39418
C	2.31035	-0.64618	1.23915
C	-0.45738	-0.49000	0.00150
P	-0.03375	1.31712	-0.02337
C	-1.90557	-0.82666	0.04857
O	0.13577	1.95505	1.29906
O	1.20130	1.38484	-1.01719
O	-1.21105	1.91786	-0.91784
C	2.46851	1.96569	-0.67702
C	-2.13629	2.90187	-0.44529
C	-2.77755	-0.06770	0.83120
C	-4.12264	-0.41028	0.90786
C	-4.60504	-1.50057	0.19097
C	-3.73623	-2.25916	-0.58941
C	-2.38895	-1.93007	-0.65445
H	2.21520	-2.15360	-1.79991
H	4.67323	-1.92358	-1.54246
H	5.61864	-0.91958	0.52001

H	4.09209	-0.11136	2.30140
H	1.63820	-0.29725	2.01524
H	2.62236	2.83125	-1.32029
H	2.48303	2.26617	0.37111
H	3.23319	1.21266	-0.86232
H	-3.13210	2.45830	-0.44732
H	-1.86895	3.23000	0.56060
H	-2.10324	3.74573	-1.13269
H	-2.39800	0.76966	1.41005
H	-4.79188	0.17106	1.53088
H	-5.65523	-1.76195	0.24364
H	-4.11034	-3.11004	-1.14606
H	-1.69751	-2.51711	-1.24653

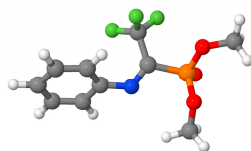
4-TS



N	-0.86748	0.23922	0.05669
C	-2.18795	0.48658	-0.01845
C	-2.82389	0.58483	-1.27042
C	-4.18754	0.82852	-1.33044
C	-4.94833	0.97248	-0.17321
C	-4.31608	0.86804	1.06228
C	-2.95306	0.62791	1.15492
C	0.35427	0.03297	0.12074
P	0.95340	-1.73064	0.10335
C	1.37877	1.12092	0.15720
O	1.69508	-2.12753	1.31797
O	-0.34668	-2.57208	-0.24937
O	1.74906	-1.85454	-1.27278
C	-1.30248	-2.89435	0.77245
C	3.17897	-1.95282	-1.30986
C	2.65739	0.89934	0.67338
C	3.58478	1.93689	0.68989
C	3.24443	3.18725	0.18664
C	1.96763	3.40968	-0.32673
C	1.03629	2.38235	-0.33636
H	-2.23602	0.46236	-2.17133
H	-4.66172	0.90210	-2.30248
H	-6.01218	1.16095	-0.23340
H	-4.88979	0.97685	1.97558
H	-2.46150	0.55424	2.11712
H	-1.80410	-3.80273	0.44781
H	-0.79684	-3.07172	1.72336
H	-2.02749	-2.08458	0.86606
H	3.60502	-0.95601	-1.43397
H	3.55473	-2.41164	-0.39446

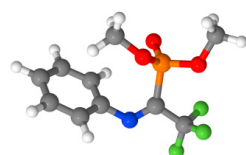
H	3.42596	-2.57255	-2.16889
H	2.91486	-0.06708	1.09418
H	4.57143	1.76816	1.10428
H	3.97071	3.99134	0.19686
H	1.70196	4.38417	-0.71839
H	0.03750	2.54095	-0.72824

5-E



N	-0.57351	0.80967	-0.04615
C	-1.96980	0.58741	-0.11733
C	-2.79151	1.31315	0.74393
C	-4.16791	1.14789	0.67694
C	-4.72906	0.30250	-0.27655
C	-3.90480	-0.38498	-1.16059
C	-2.52377	-0.25157	-1.08363
C	0.28342	-0.10141	0.11657
P	2.03674	0.44374	0.16414
C	-0.00358	-1.58624	0.37534
F	-1.11038	-1.77008	1.09252
F	-0.13691	-2.26023	-0.77376
F	1.00910	-2.13282	1.05014
O	2.58544	0.61846	1.51836
O	2.69651	-0.66088	-0.76557
O	2.08462	1.74385	-0.75242
C	4.12708	-0.77105	-0.83008
C	1.85039	3.04629	-0.19316
H	-2.33983	1.98253	1.46583
H	-4.80545	1.69260	1.36273
H	-5.80435	0.18815	-0.33569
H	-4.33555	-1.03263	-1.91456
H	-1.87691	-0.77969	-1.77359
H	4.33681	-1.67176	-1.40024
H	4.54230	0.09931	-1.34048
H	4.53999	-0.85433	0.17579
H	0.77689	3.22780	-0.15228
H	2.28858	3.11153	0.80352
H	2.32933	3.75757	-0.86178

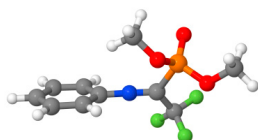
5-Z



N	-0.32002	-1.53739	-0.07240
C	-1.62599	-1.00551	0.00891
C	-2.49853	-1.22551	-1.05859
C	-3.80388	-0.76076	-0.98132

C	-4.25670	-0.11896	0.17088
C	-3.39141	0.06512	1.24302
C	-2.07136	-0.36935	1.16823
C	0.71086	-0.82360	0.03932
P	0.74149	1.02088	0.21169
C	2.05389	-1.55736	0.01692
F	1.90294	-2.86390	0.19046
F	2.68562	-1.37096	-1.14516
F	2.84432	-1.10218	0.99682
O	0.44603	1.55535	1.55193
O	2.19329	1.28655	-0.37082
O	-0.22095	1.54121	-0.94589
C	2.73818	2.61328	-0.34065
C	-1.44354	2.25666	-0.69821
H	-2.13805	-1.75086	-1.93438
H	-4.47631	-0.91618	-1.81645
H	-5.28227	0.22350	0.23412
H	-3.73857	0.55113	2.14692
H	-1.39220	-0.22556	2.00014
H	3.76568	2.52723	-0.68268
H	2.17464	3.26032	-1.01553
H	2.70940	3.00616	0.67633
H	-2.27844	1.62265	-0.99390
H	-1.52278	2.51901	0.35682
H	-1.41538	3.15550	-1.31182

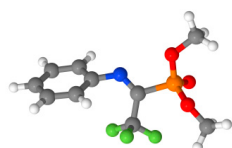
5-TS



N	-0.74767	0.35866	-0.00201
C	-2.08582	0.13436	-0.04996
C	-2.62407	-0.63832	-1.09059
C	-3.99355	-0.85571	-1.13877
C	-4.82958	-0.36226	-0.14139
C	-4.28334	0.37999	0.90195
C	-2.92435	0.65454	0.94643
C	0.46310	0.57481	0.03527
P	1.64569	-0.82013	0.32964
C	1.03120	1.99891	-0.11137
F	2.08396	2.17159	0.69185
F	1.43028	2.21813	-1.36692
F	0.11388	2.91243	0.19481
O	2.00928	-1.04016	1.73894
O	0.91996	-2.05890	-0.37059
O	2.80945	-0.45920	-0.68571
C	0.03709	-2.90610	0.38397
C	4.05976	-1.16562	-0.62257
H	-1.96108	-1.03876	-1.84786
H	-4.40656	-1.43383	-1.95689
H	-5.89450	-0.55281	-0.17725

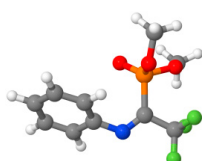
H	-4.92428	0.77075	1.68329
H	-2.49589	1.25564	1.73816
H	-0.95820	-2.45879	0.41897
H	0.42445	-3.04949	1.39310
H	-0.00284	-3.85606	-0.14360
H	4.73436	-0.64790	-1.29861
H	4.44962	-1.14214	0.39543
H	3.91806	-2.19603	-0.95190

5'-E



N	-0.66554	0.91649	0.08336
C	-2.05369	0.67081	-0.01674
C	-2.89181	1.28730	0.91194
C	-4.26399	1.09927	0.82528
C	-4.80667	0.34501	-0.21188
C	-3.96773	-0.22813	-1.16138
C	-2.59000	-0.07434	-1.06701
C	0.21460	0.01707	0.12507
P	1.97822	0.53283	0.20814
C	-0.03393	-1.49455	0.20169
F	0.99679	-2.08401	0.82735
F	-1.13549	-1.80324	0.87655
F	-0.12137	-2.04279	-1.01651
O	2.55044	0.62427	1.56128
O	2.72139	-0.50072	-0.75947
O	1.92334	1.86438	-0.64768
C	3.62461	-1.50613	-0.27180
C	3.06470	2.73340	-0.64427
H	-2.45371	1.89231	1.69609
H	-4.91361	1.55777	1.56099
H	-5.87930	0.21508	-0.28571
H	-4.38448	-0.80107	-1.98088
H	-1.93248	-0.51095	-1.80914
H	3.19484	-2.48253	-0.48825
H	3.78051	-1.39007	0.80089
H	4.56633	-1.38451	-0.80414
H	2.76444	3.62986	-1.17968
H	3.34650	2.97996	0.37994
H	3.89932	2.25480	-1.16060

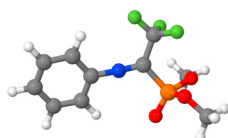
5'-Z



N	-0.64461	1.44231	-0.24804
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C	-1.89876	0.80760	-0.11344
C	-2.80735	1.34446	0.79736
C	-4.05618	0.75789	0.94084
C	-4.42000	-0.32416	0.14320
C	-3.52565	-0.82275	-0.79721
C	-2.26052	-0.26449	-0.92801
C	0.44678	0.81502	-0.19850
P	0.69338	-0.96209	0.26136
C	1.71546	1.63297	-0.43378
F	1.45746	2.84200	-0.90712
F	2.39674	1.78338	0.71613
F	2.52146	1.01024	-1.30007
O	-0.25937	-1.47903	1.25323
O	0.74408	-1.64007	-1.17642
O	2.22418	-1.04489	0.71468
C	1.13300	-3.01967	-1.28994
C	2.57400	-0.99011	2.10781
H	-2.51445	2.20122	1.39142
H	-4.75415	1.15620	1.66721
H	-5.40222	-0.76857	0.24713
H	-3.81116	-1.65233	-1.43265
H	-1.56103	-0.63942	-1.66629
H	1.00708	-3.28495	-2.33600
H	2.17750	-3.13149	-0.99748
H	0.49135	-3.64289	-0.66512
H	2.48617	0.03430	2.47097
H	1.92643	-1.65114	2.68324
H	3.60931	-1.31494	2.17110

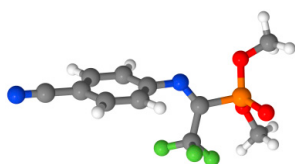
5'-TS



N	0.91544	0.13477	-0.05906
C	2.25325	-0.13002	-0.02689
C	2.68579	-1.39077	0.41156
C	4.04367	-1.66679	0.47075
C	4.96812	-0.70989	0.05649
C	4.54035	0.53554	-0.40031
C	3.18726	0.83790	-0.42559
C	-0.28074	0.43568	-0.07849
P	-1.55737	-0.89816	-0.00691
C	-0.76086	1.89582	-0.08368
F	-1.75861	2.08708	-0.94924
F	-1.21361	2.24558	1.13347
F	0.23037	2.72952	-0.39779
O	-1.02734	-2.15565	0.54829
O	-2.81679	-0.29156	0.78312
O	-2.10527	-0.91960	-1.49900
C	-2.84867	-0.36945	2.21477
C	-3.17267	-1.81551	-1.84339
H	1.93292	-2.11654	0.69771

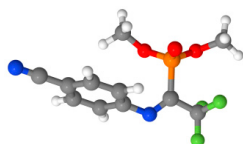
H	4.38335	-2.63362	0.82152
H	6.02747	-0.93574	0.08834
H	5.26495	1.27408	-0.72086
H	2.82614	1.80488	-0.75379
H	-2.66769	-1.39431	2.53989
H	-3.84052	-0.04272	2.51662
H	-2.09884	0.29891	2.64352
H	-3.30826	-1.72920	-2.91806
H	-2.90287	-2.83961	-1.58069
H	-4.08539	-1.51749	-1.32555

6-E



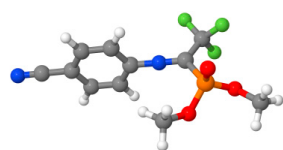
N	-0.10307	0.88789	-0.02692
C	0.75677	-0.02895	-0.09159
P	2.53953	0.39179	-0.27371
C	0.45144	-1.53348	-0.06428
F	0.14440	-1.99528	-1.27641
F	-0.55215	-1.82412	0.76086
F	1.53054	-2.20222	0.36565
O	3.16011	-0.26305	-1.43620
O	2.46818	1.96964	-0.24239
O	3.21768	0.03867	1.12779
C	3.68662	2.72117	-0.35183
C	4.06505	-1.10931	1.30771
C	-1.49514	0.66264	-0.00006
C	-2.21821	1.14148	1.09361
C	-3.59135	0.97762	1.13185
C	-4.25224	0.37619	0.05626
C	-3.52992	-0.06312	-1.05421
C	-2.15108	0.07550	-1.08298
C	-5.67952	0.22270	0.08982
N	-6.82294	0.10030	0.11879
H	4.30401	2.55485	0.53251
H	4.22735	2.43264	-1.25438
H	3.39334	3.76554	-0.40950
H	4.32245	-1.54645	0.34285
H	4.96269	-0.76577	1.81801
H	3.53810	-1.83519	1.92429
H	-1.69121	1.62567	1.90586
H	-4.16145	1.32512	1.98408
H	-4.05049	-0.51543	-1.88880
H	-1.58313	-0.25726	-1.94272

6-Z



N	-0.21444	-1.55407	0.00108
C	1.11739	-1.09499	0.04508
C	1.97103	-1.43188	-1.00778
C	3.29574	-1.03341	-0.97052
C	3.78246	-0.33101	0.13804
C	2.93372	-0.02578	1.20328
C	1.59892	-0.40155	1.15728
C	-1.19662	-0.76702	0.02611
P	-1.12821	1.08691	0.04890
C	-2.58659	-1.39613	0.05035
F	-2.56165	-2.67673	0.37954
F	-3.35002	-0.74935	0.95001
F	-3.18431	-1.28173	-1.13833
O	-0.84778	1.65538	1.37841
O	-0.07188	1.36250	-1.09626
O	-2.50539	1.49522	-0.61767
C	1.09869	2.17942	-0.91320
C	-3.59357	2.08648	0.11745
C	5.15990	0.07290	0.17934
N	6.26213	0.40085	0.20765
H	1.58056	-1.99370	-1.84674
H	3.96361	-1.27297	-1.78840
H	3.31916	0.51029	2.06153
H	0.93036	-0.15952	1.97455
H	1.96364	1.56945	-1.17103
H	1.01971	3.02958	-1.58807
H	1.17000	2.51769	0.12079
H	-4.44476	1.41259	0.04864
H	-3.31105	2.23968	1.15910
H	-3.82395	3.03917	-0.35452

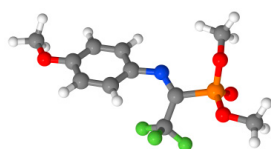
6-TS



N	-0.19319	0.41932	0.02956
C	1.02800	0.57036	0.05735
C	1.66635	1.97120	-0.00505
F	0.77627	2.91403	0.28248
F	2.14336	2.20625	-1.22855
F	2.67585	2.05910	0.86148
P	2.12184	-0.91244	0.26112
O	3.35620	-0.50350	-0.63974
C	4.56925	-1.27746	-0.60004
H	5.30574	-0.71208	-1.16355
H	4.40092	-2.24733	-1.06967
H	4.89548	-1.40378	0.43254

O	1.38227	-2.02885	-0.60209
C	0.41418	-2.90769	-0.00084
H	0.70564	-3.14450	1.02272
H	0.39881	-3.80926	-0.60796
H	-0.56770	-2.43161	-0.01704
O	2.36919	-1.27579	1.66464
C	-1.53199	0.28236	0.00268
C	-2.19943	0.14309	-1.22746
C	-2.25736	0.24558	1.20738
C	-3.57054	-0.02635	-1.24166
C	-3.62761	0.07595	1.17045
C	-4.29854	-0.06237	-0.04874
H	-1.63161	0.17137	-2.14801
H	-1.73351	0.35154	2.14813
H	-4.08819	-0.13205	-2.18701
H	-4.18964	0.04906	2.09576
C	-5.71967	-0.24229	-0.07544
N	-6.86111	-0.38907	-0.09750

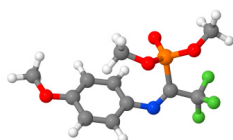
7-E



N	0.03169	0.69006	-0.03593
C	-1.34702	0.40512	-0.11549
C	-2.21107	1.27558	0.54052
C	-3.58734	1.08355	0.49505
C	-4.10922	0.04094	-0.27092
C	-3.24513	-0.80138	-0.97897
C	-1.87841	-0.62902	-0.89684
C	0.96104	-0.15342	0.11201
P	2.65471	0.54920	0.16631
C	0.82061	-1.65701	0.36833
F	-0.27459	-1.95377	1.06780
F	0.77775	-2.35099	-0.77787
F	1.87074	-2.09657	1.06426
O	3.18051	0.79530	1.51929
O	3.42599	-0.49946	-0.74421
O	2.59474	1.83801	-0.76836
C	4.86003	-0.46848	-0.79888
C	2.24642	3.12106	-0.22713
O	-5.43021	-0.22299	-0.40441
C	-6.34333	0.60715	0.28477
H	-1.79208	2.09714	1.10891
H	-4.23341	1.75859	1.03889
H	-3.67565	-1.58619	-1.58803
H	-1.22004	-1.27920	-1.45941
H	5.16268	-1.35427	-1.35057
H	5.19087	0.42924	-1.32359
H	5.27260	-0.49156	0.21043
H	1.16095	3.21088	-0.19492

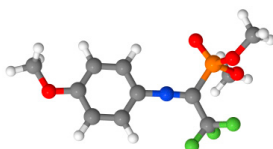
H	2.66942	3.23552	0.77178
H	2.66764	3.86355	-0.90089
H	-6.26458	1.64491	-0.05310
H	-6.18017	0.55954	1.36565
H	-7.33347	0.22401	0.05053

7-Z



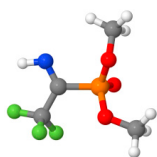
N	0.35087	-1.56803	0.01024
C	-0.99278	-1.13154	0.02700
C	-1.83075	-1.59178	1.04939
C	-3.15930	-1.21824	1.07546
C	-3.69117	-0.42466	0.05042
C	-2.87070	-0.00305	-0.99258
C	-1.51974	-0.35037	-0.99560
C	1.31417	-0.75872	-0.06148
P	1.22567	1.09284	0.00338
C	2.71024	-1.36352	-0.17076
F	2.68789	-2.63497	-0.53952
F	3.42349	-0.68162	-1.08843
F	3.37171	-1.28172	0.98757
O	0.85429	1.74814	-1.26367
O	0.27195	1.32332	1.24657
O	2.64995	1.47214	0.59172
C	-0.97101	2.04048	1.17432
C	3.67121	2.12134	-0.18437
O	-5.01067	-0.13147	0.15703
C	-5.59422	0.65298	-0.86350
H	-1.41836	-2.22846	1.82244
H	-3.82007	-1.54529	1.86858
H	-3.25776	0.59277	-1.80777
H	-0.88269	-0.01956	-1.80725
H	-1.77367	1.34215	1.40971
H	-0.92918	2.83719	1.91482
H	-1.11458	2.45521	0.17616
H	4.53870	1.46499	-0.20637
H	3.31626	2.31681	-1.19651
H	3.91632	3.05709	0.31427
H	-6.64035	0.77072	-0.59162
H	-5.52356	0.15273	-1.83407
H	-5.11999	1.63748	-0.92426

7-TS



N	0.20565	0.32841	-0.09525
C	-1.02232	0.47545	-0.10380
C	-1.68304	1.85983	-0.11294
F	-0.81812	2.80689	-0.48067
F	-2.12714	2.17941	1.11745
F	-2.73289	1.91172	-0.93594
P	-2.10567	-1.01069	0.00099
O	-2.76322	-1.07550	-1.44631
C	-3.73866	-2.08874	-1.72913
H	-3.96625	-2.00626	-2.78856
H	-4.63798	-1.91023	-1.13800
H	-3.32969	-3.07646	-1.50982
O	-3.37464	-0.59838	0.89766
C	-3.26596	-0.66784	2.32487
H	-2.92183	-1.65709	2.62854
H	-4.26052	-0.47303	2.71821
H	-2.57546	0.09747	2.68701
O	-1.38005	-2.20430	0.47204
C	1.56008	0.24491	-0.08198
C	2.16660	-1.00163	0.12336
C	2.37066	1.38350	-0.26407
C	3.54752	-1.12248	0.15601
C	3.74220	1.26822	-0.24978
C	4.33834	0.01555	-0.03622
H	1.51985	-1.86094	0.26325
H	1.89052	2.34188	-0.42084
H	3.99412	-2.09265	0.32350
H	4.38836	2.12480	-0.39433
O	5.68597	0.00790	-0.03304
C	6.35002	-1.22578	0.17148
H	6.10007	-1.64813	1.14876
H	6.09752	-1.94162	-0.61573
H	7.41304	-1.00210	0.13286

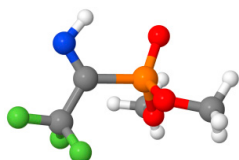
8-E



N	-0.61024	-2.04384	-0.24099
C	-0.65754	-0.79852	-0.06136
P	0.93126	0.06675	0.25283
C	-1.95733	0.00364	-0.01913
F	-1.96725	0.84417	1.01305
F	-2.11742	0.71024	-1.13754
F	-3.01257	-0.81185	0.09752
O	1.30799	0.12083	1.67310
O	0.65186	1.43914	-0.49033
O	1.98241	-0.65137	-0.69983
C	1.57628	2.52947	-0.34513
C	2.72091	-1.79835	-0.24203

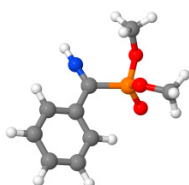
H	-1.54565	-2.45100	-0.33565
H	2.51132	2.28983	-0.85344
H	1.75700	2.72632	0.71212
H	1.10675	3.38921	-0.81468
H	2.09479	-2.68540	-0.33100
H	3.58939	-1.87902	-0.89082
H	3.03232	-1.65371	0.79291

8-Z



N	1.18100	0.09518	-2.02767
C	0.78546	-0.05925	-0.84327
C	1.82340	-0.24037	0.25623
P	-0.99767	0.05357	-0.40674
F	3.01540	-0.56370	-0.21799
F	1.94614	0.91195	0.93899
F	1.44560	-1.18006	1.12634
O	-1.75532	0.55737	-1.56432
O	-1.31400	-1.39690	0.13558
O	-1.09266	0.93388	0.92050
C	-2.61041	-1.69884	0.68046
C	-1.03649	2.36674	0.82230
H	0.37835	0.26334	-2.64539
H	-2.60679	-2.76397	0.89303
H	-3.38685	-1.46412	-0.04894
H	-2.76244	-1.13181	1.59924
H	-1.25799	2.74787	1.81533
H	-0.03301	2.67911	0.52550
H	-1.77337	2.72168	0.10162

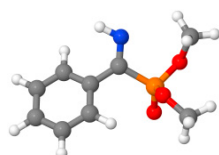
8-TS



N	-0.77258	-2.13666	-0.27547
C	-0.69255	-0.93514	-0.04240
C	-1.94474	-0.04042	-0.01218
P	0.92550	-0.06992	0.29183
F	-3.02979	-0.73677	0.29104
F	-1.80631	0.95061	0.87540
F	-2.13270	0.52019	-1.21262
O	1.17833	0.34170	1.68754
O	1.91453	-1.15626	-0.33873
O	1.02301	1.12441	-0.78093
C	3.30599	-0.85150	-0.30058

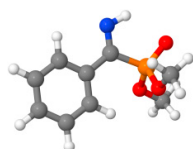
C	0.81320	2.47727	-0.37252
H	-0.86350	-3.10990	-0.45716
H	3.79504	-1.51327	-1.01891
H	3.70216	-1.02737	0.70588
H	3.48968	0.19124	-0.58913
H	1.26263	3.10667	-1.14466
H	-0.25421	2.70373	-0.29940
H	1.29455	2.66819	0.59296

9-E



N	0.30427	2.07420	0.55641
C	-0.04916	0.92715	0.14203
P	1.31376	-0.13074	-0.49320
C	-1.43783	0.39438	0.09882
C	-1.68852	-0.97103	0.24807
C	-2.99485	-1.44411	0.24293
C	-4.05730	-0.56415	0.06745
O	1.02387	-0.86817	-1.73019
O	1.57578	-1.05219	0.80509
O	2.60084	0.79374	-0.61433
C	2.43295	-2.19324	0.65636
C	3.26550	1.42467	0.48811
C	-3.81236	0.79508	-0.10576
C	-2.50895	1.27177	-0.08982
H	-0.50125	2.60170	0.90486
H	-0.86412	-1.66182	0.37764
H	-3.18214	-2.50346	0.36872
H	-5.07427	-0.93752	0.05324
H	3.45710	-1.87341	0.44983
H	2.07650	-2.82683	-0.15721
H	2.39824	-2.73112	1.60055
H	3.05953	0.89534	1.42037
H	4.33138	1.38940	0.26835
H	2.91864	2.45191	0.56692
H	-4.63552	1.48074	-0.26596
H	-2.32103	2.32678	-0.25793

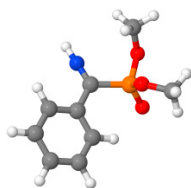
9-Z



N	-0.02082	2.23291	-0.86882
C	-0.06460	1.02712	-0.47193
P	1.55037	0.20229	-0.15554

C	-1.36243	0.34494	-0.22460
C	-1.43516	-0.97743	0.21834
C	-2.67345	-1.57218	0.44183
C	-3.84302	-0.85540	0.22396
O	2.67525	1.12065	-0.41680
O	1.48930	-1.13775	-1.00966
O	1.50443	-0.37769	1.34259
C	2.66995	-1.94975	-1.11999
C	1.66968	0.54111	2.43090
C	-3.77577	0.46445	-0.22034
C	-2.54524	1.06128	-0.44286
H	0.94926	2.54258	-0.97648
H	-0.53283	-1.55026	0.38911
H	-2.72045	-2.59852	0.78518
H	-4.80586	-1.32121	0.39803
H	2.89678	-2.40514	-0.15478
H	3.51046	-1.34295	-1.45897
H	2.44222	-2.71961	-1.85214
H	0.81499	1.22117	2.48096
H	1.71185	-0.05779	3.33691
H	2.59246	1.10909	2.30693
H	-4.68611	1.02609	-0.39265
H	-2.47414	2.08515	-0.78810

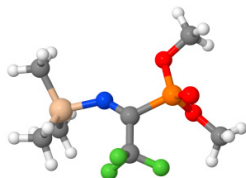
9-TS



N	0.26426	2.20445	-0.29294
C	-0.01542	0.99975	-0.28519
P	1.37403	-0.23863	-0.46407
C	-1.39880	0.44626	-0.11811
C	-1.71196	-0.86608	-0.47737
C	-3.01142	-1.33681	-0.31721
C	-3.99607	-0.50963	0.21024
O	1.32570	-1.17003	-1.60393
O	1.32220	-0.93605	0.98782
O	2.71465	0.63092	-0.45911
C	2.01998	-2.17313	1.18407
C	3.13169	1.42296	0.65392
C	-3.68501	0.79988	0.57235
C	-2.39345	1.27548	0.40407
H	0.48535	3.17042	-0.34514
H	-0.95487	-1.51150	-0.90868
H	-3.25351	-2.35152	-0.60925
H	-5.00565	-0.88193	0.33871
H	3.09903	-2.01558	1.11595
H	1.70962	-2.90196	0.43438
H	1.75924	-2.51981	2.18094
H	2.46012	1.30554	1.50632

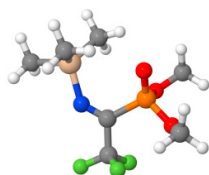
H	4.13435	1.10034	0.93522
H	3.15296	2.46629	0.34253
H	-4.45066	1.44539	0.98599
H	-2.13394	2.29200	0.67579

10-E



N	-0.88482	-0.70726	0.01331
C	0.04561	0.11239	-0.11081
C	-0.16683	1.63260	-0.20398
P	1.80787	-0.41926	-0.27413
F	-1.10513	2.03519	0.66339
F	0.95794	2.29993	0.08544
F	-0.55975	1.99994	-1.42341
O	2.46176	0.05503	-1.50706
O	2.54062	0.04627	1.07296
O	1.66488	-1.98247	-0.06435
C	3.45609	1.15190	1.10426
C	2.84493	-2.79248	-0.14095
Si	-2.66312	-0.62673	0.14232
C	-3.01724	-0.35773	1.95719
C	-3.23905	-2.30773	-0.42659
C	-3.41344	0.69687	-0.94943
H	4.34186	0.81966	1.64281
H	2.98577	1.97899	1.63369
H	3.72270	1.45452	0.09131
H	2.51187	-3.82373	-0.06149
H	3.35070	-2.63386	-1.09470
H	3.51453	-2.55332	0.68749
H	-2.67718	0.62711	2.28250
H	-2.51695	-1.11464	2.56520
H	-4.09155	-0.42905	2.14663
H	-2.78461	-3.09354	0.18038
H	-2.95706	-2.48383	-1.46743
H	-4.32584	-2.39766	-0.35175
H	-3.02941	0.62670	-1.97019
H	-3.22500	1.70660	-0.58369
H	-4.49645	0.54881	-0.99389

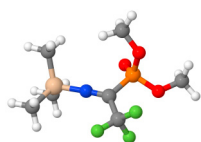
10-Z



N	1.08162	1.01627	-0.09398
C	-0.14169	0.77664	-0.12318

C	-1.13468	1.91993	-0.36156
P	-0.87357	-0.90331	0.14351
F	-0.53475	3.06587	-0.63635
F	-1.96012	1.62407	-1.37235
F	-1.89479	2.10541	0.73513
O	-0.14716	-1.68063	1.16667
O	-2.43398	-0.72594	0.42998
O	-0.85502	-1.46438	-1.34299
C	-2.92644	-0.67278	1.77939
C	-1.22045	-2.83255	-1.58255
Si	2.54200	0.00434	0.15705
C	2.71572	-0.21072	2.00139
C	3.92066	1.04561	-0.55242
C	2.43376	-1.61510	-0.77812
H	-2.69494	0.29736	2.22000
H	-2.48319	-1.47305	2.37182
H	-4.00388	-0.79810	1.71150
H	-1.06654	-3.00683	-2.64391
H	-0.58457	-3.49686	-0.99530
H	-2.27005	-2.98693	-1.32757
H	1.89802	-0.82563	2.38146
H	2.70450	0.75573	2.51048
H	3.66383	-0.70279	2.23478
H	3.96516	2.01700	-0.05522
H	3.76671	1.22302	-1.61964
H	4.88802	0.55163	-0.42885
H	2.01722	-1.46569	-1.77773
H	1.81926	-2.34139	-0.24512
H	3.43947	-2.02917	-0.89483

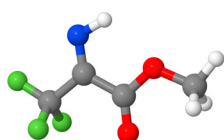
10-TS



N	-1.04542	0.12266	0.06071
C	0.12992	0.50066	0.02995
C	0.51590	1.95852	-0.27951
P	1.46004	-0.75310	0.30455
F	1.04401	2.54978	0.79660
F	1.41773	2.01429	-1.26557
F	-0.54725	2.66664	-0.65405
O	1.08525	-1.80934	1.25782
O	1.80358	-1.30019	-1.16616
O	2.72609	0.14750	0.62151
C	1.01676	-2.36592	-1.71248
C	4.01106	-0.45996	0.82320
Si	-2.71241	-0.34499	0.18696
C	-2.90682	-1.88183	-0.86060
C	-3.84154	1.01282	-0.42558
C	-2.95083	-0.68020	2.00675
H	0.02315	-1.99728	-1.97944
H	0.92855	-3.17820	-0.99014

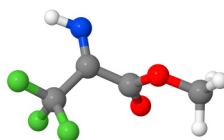
H	1.53437	-2.70463	-2.60658
H	4.68076	0.33922	1.12845
H	3.94818	-1.21710	1.60611
H	4.35795	-0.90462	-0.11038
H	-2.24441	-2.67311	-0.50188
H	-2.67310	-1.67924	-1.90902
H	-3.93577	-2.24897	-0.81827
H	-3.63645	1.24791	-1.47284
H	-3.69688	1.92677	0.15519
H	-4.89218	0.72018	-0.34474
H	-2.78488	0.22409	2.59639
H	-2.24665	-1.44337	2.34456
H	-3.96818	-1.02842	2.20332

11-E



C	1.51622	-0.11407	0.00001
F	2.56540	0.69578	-0.00023
F	1.59478	-0.89383	1.08230
F	1.59449	-0.89412	-1.08211
C	0.20712	0.66872	0.00008
C	-1.04830	-0.18714	0.00004
O	-1.04093	-1.38233	-0.00004
O	-2.13956	0.57679	0.00014
C	-3.38517	-0.13445	-0.00006
N	0.24150	1.92390	-0.00006
H	-4.15808	0.62806	-0.00145
H	-3.45522	-0.75867	0.89018
H	-3.45387	-0.76064	-0.88900
H	-0.71057	2.29929	-0.00016

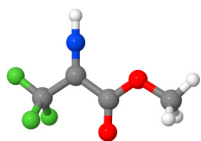
11-Z



C	1.48509	-0.15349	-0.00006
F	2.55301	0.65752	-0.00004
F	1.56670	-0.92364	1.08184
F	1.56661	-0.92345	-1.08209
C	0.19939	0.67778	0.00008
C	-1.07327	-0.14647	0.00045
O	-1.05513	-1.34605	0.00017
O	-2.15803	0.60758	0.00005
C	-3.39635	-0.11245	-0.00028
N	0.17418	1.93339	0.00011
H	-4.17303	0.64619	-0.00114

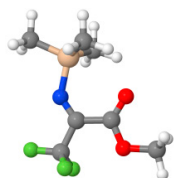
H	-3.46487	-0.73871	0.88909
H	-3.46385	-0.73972	-0.88901
H	1.12174	2.32023	-0.00005

11-TS



C	1.50266	-0.14524	0.00009
F	2.57295	0.64463	0.00043
F	1.56885	-0.92353	1.08348
F	1.56944	-0.92339	-1.08336
C	0.20616	0.70136	-0.00017
C	-1.06650	-0.15892	-0.00019
O	-1.04376	-1.35699	-0.00056
O	-2.16108	0.58911	0.00026
C	-3.39170	-0.14265	0.00024
N	0.22480	1.92223	-0.00035
H	-4.17803	0.60629	0.00097
H	-3.45318	-0.77142	0.88846
H	-3.45379	-0.77031	-0.88872
H	0.24516	2.91610	-0.00057

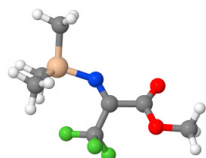
12-E



C	1.63340	-1.41196	0.00007
F	1.17275	-2.65442	0.00089
F	2.40896	-1.26551	-1.08324
F	2.40964	-1.26433	1.08276
C	0.48750	-0.38747	-0.00005
C	0.88994	1.08875	0.00067
O	0.07680	1.97161	0.00315
O	2.20180	1.26323	-0.00175
C	2.65065	2.62409	-0.00090
N	-0.69120	-0.78892	-0.00035
C	-2.49716	1.00400	1.57471
C	-3.49873	-1.40861	-0.00420
C	-2.49556	1.01085	-1.57110
Si	-2.29096	0.01754	-0.00022
H	3.73507	2.57313	-0.00174
H	2.28500	3.13488	0.88950
H	2.28376	3.13636	-0.88996
H	-1.88834	1.90759	1.56998
H	-2.22635	0.40033	2.44478
H	-3.54661	1.29012	1.68884

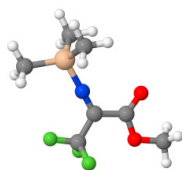
H	-3.35774	-2.03975	0.87644
H	-3.35681	-2.03562	-0.88766
H	-4.53193	-1.05102	-0.00396
H	-2.21861	0.41276	-2.44311
H	-1.89092	1.91716	-1.55972
H	-3.54589	1.29261	-1.68791

12-Z



C	0.67738	1.32432	0.11416
F	0.96657	1.78980	-1.10298
F	-0.46605	1.90384	0.50292
F	1.63112	1.73131	0.95610
C	0.53226	-0.20812	0.12507
C	1.84433	-0.99045	0.19966
O	1.96010	-2.05535	0.72640
O	2.81781	-0.33333	-0.43226
C	4.09535	-0.97958	-0.43732
N	-0.54921	-0.82106	0.07240
C	-2.86964	0.15468	1.59741
C	-3.08802	-2.04205	-0.53642
C	-2.56066	0.82132	-1.45045
Si	-2.28012	-0.42305	-0.07922
H	4.75835	-0.31603	-0.98442
H	4.02116	-1.94880	-0.93009
H	4.44421	-1.12056	0.58555
H	-2.44564	1.12315	1.86552
H	-2.59591	-0.56916	2.36867
H	-3.95936	0.24413	1.59702
H	-2.88507	-2.79996	0.22339
H	-2.70303	-2.41434	-1.48883
H	-4.17141	-1.93014	-0.63032
H	-2.02723	0.52055	-2.35625
H	-2.23839	1.82738	-1.18163
H	-3.62566	0.85820	-1.69657

12-TS



C	-1.13393	-1.50747	0.00000
F	-0.17673	-2.43277	-0.00000
F	-1.89348	-1.71128	1.08291
F	-1.89349	-1.71128	-1.08290

C	-0.51743	-0.09350	0.00000
C	-1.48967	1.09628	0.00000
O	-1.12102	2.23375	0.00002
O	-2.75890	0.70006	-0.00001
C	-3.73512	1.74708	-0.00001
N	0.70120	0.08017	0.00000
C	2.79404	1.26857	1.55664
C	2.79403	1.26859	-1.55664
C	3.30989	-1.33829	-0.00002
Si	2.42080	0.30638	-0.00000
H	-4.69992	1.24888	0.00000
H	-3.61679	2.36612	-0.88916
H	-3.61677	2.36613	0.88914
H	2.48459	0.71335	2.44513
H	2.26759	2.22501	1.54913
H	3.86685	1.46139	1.64027
H	2.26759	2.22503	-1.54910
H	2.48455	0.71339	-2.44513
H	3.86684	1.46140	-1.64028
H	3.04130	-1.92420	-0.88233
H	3.04134	-1.92420	0.88230
H	4.39507	-1.20287	-0.00004