Electronic supplementary information -1 for

Anharmonicity and Vibrational Stark Fields in Phosphinic Acid Dimers

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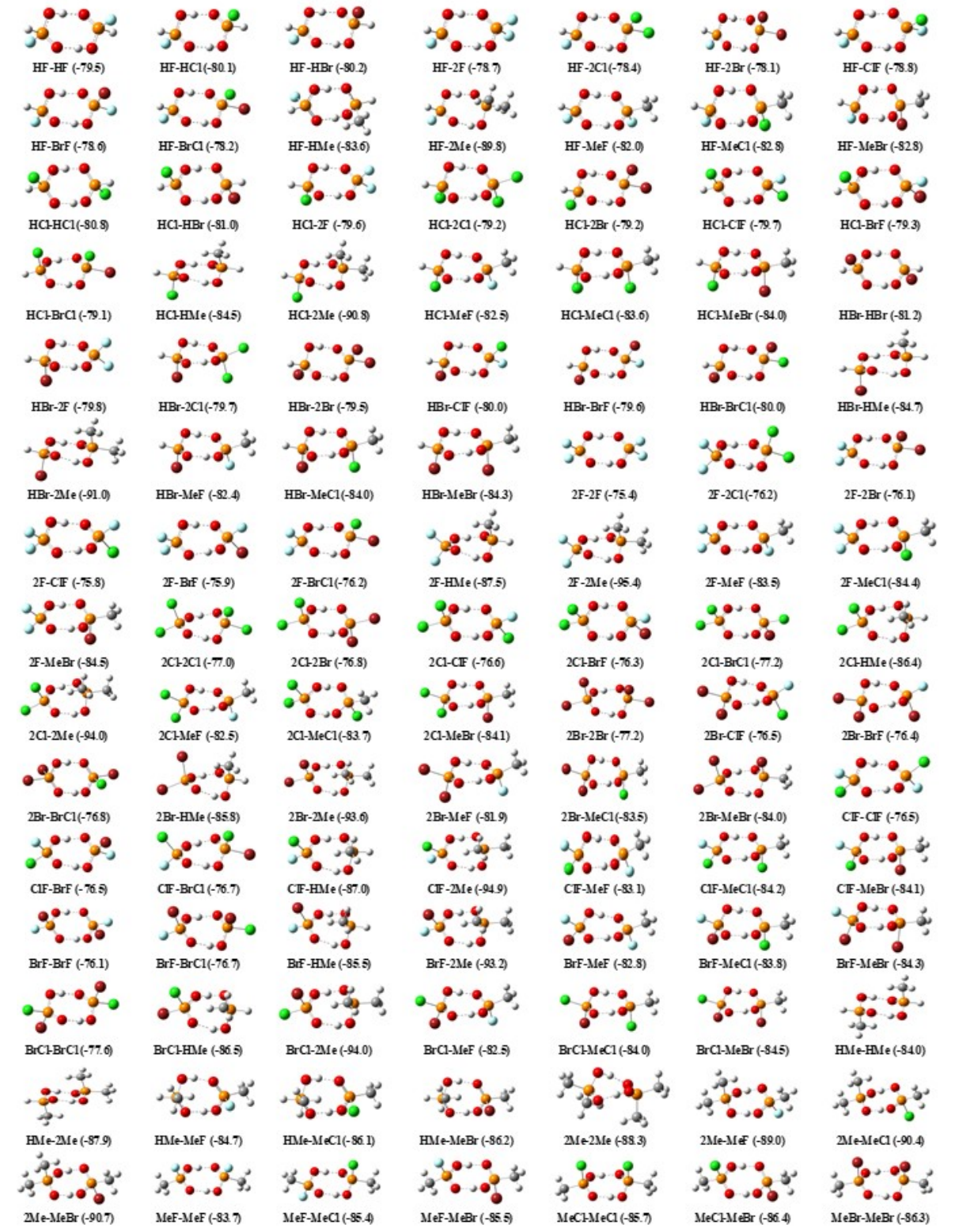

Figure S1 Optimized Structures of all possible phosphinic acid dimers with –R groups as –H, -Me, -F, -Cl, -Br with their ZPE and BSSE corrected stabilization energies (in kJ mol^{-1}) calculated at the MP2/aug-cc-pVDZ level of theory shown in the parentheses. For the sake of convenience, the different possible dimers formed by different combinations of the monomeric units will be labelled with respect to the R groups as R_1R_2, i.e., dimer formed by combination of PA-2H and PA-BrCl will be labelled as (2H-

BrCl).

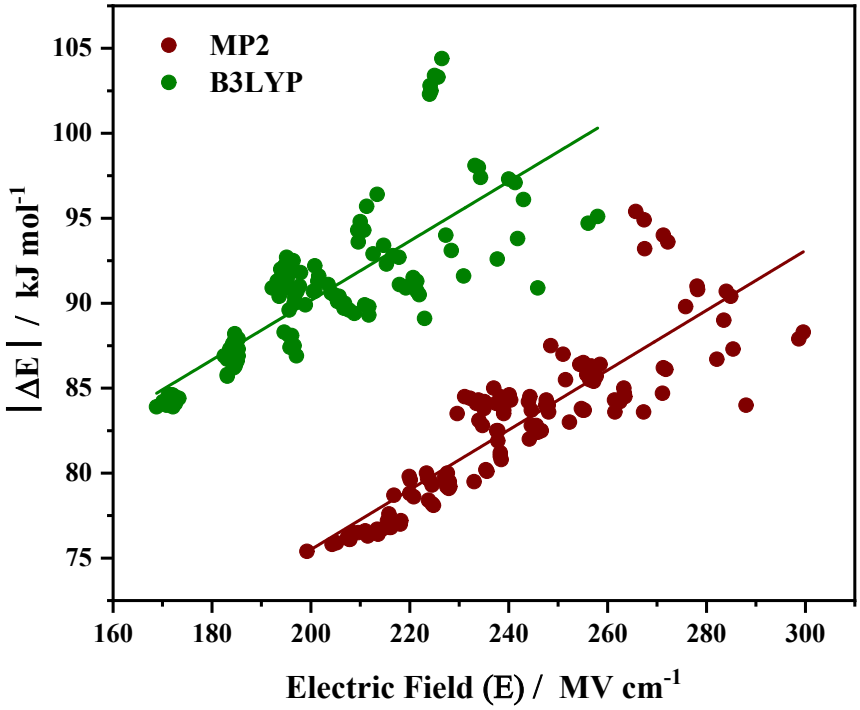

Figure S2. Plots of stabilization energy of various phosphinic acid dimer against the corresponding total electric field calculated at MP2 (brown circles) and B3LYP-D3 (green circles). The straight-lines are linear least-square fits to the data.

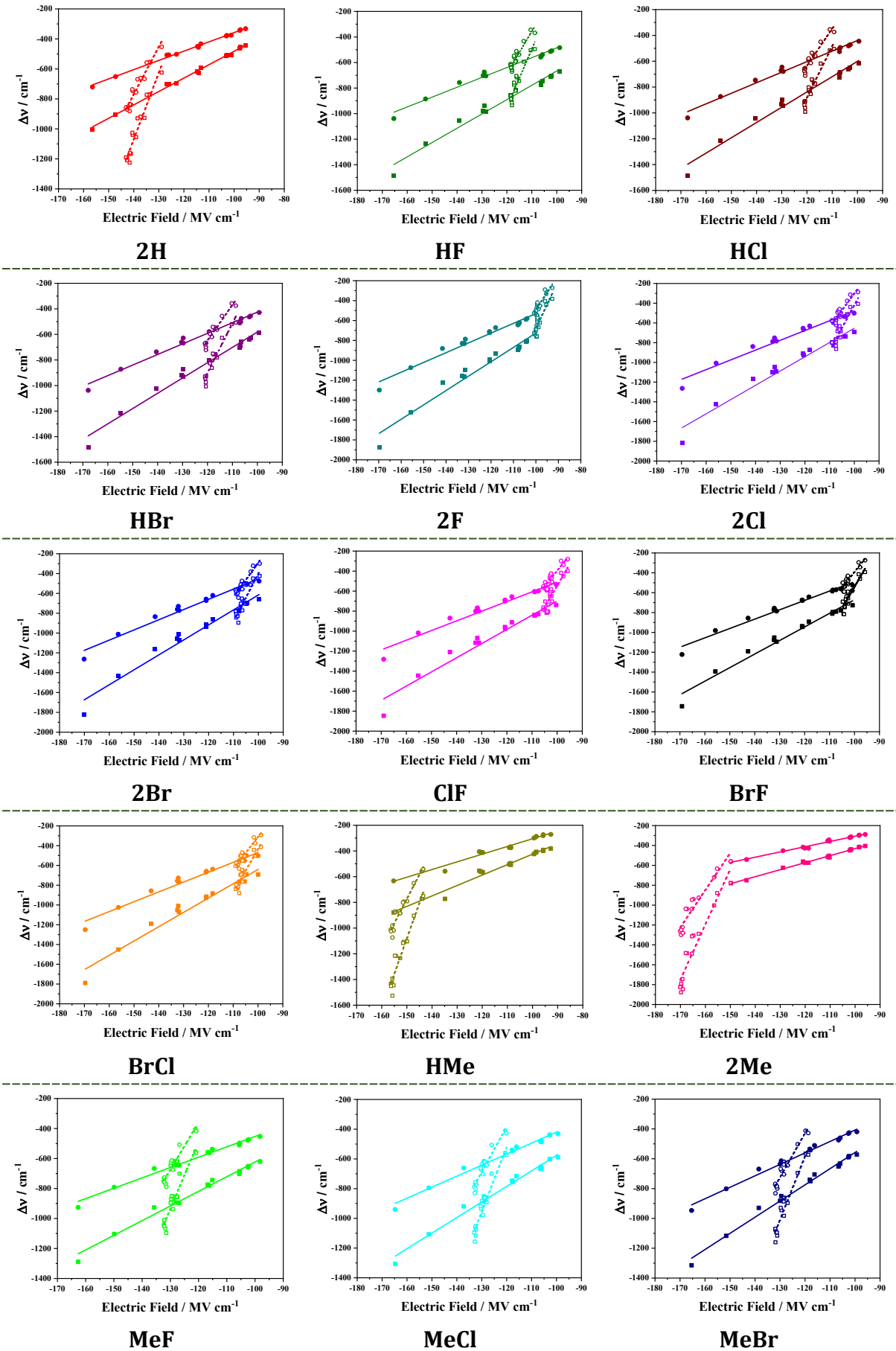
Δν / cm-1
Electric Field / MV cm-1
2H
HF
HCl
HBr
2F
2Cl
2Br
ClF
BrF
BrCl
HMe
2Me
MeF
MeCl
MeBr

Figure S3. Plots of the red-shifts in the O–H (squares) and O–D (circles) stretching frequencies against the corresponding Stark fields in the dimers of 2H, HF, HCl, HBr, 2F, 2Cl, 2Br, ClF, BrF, BrCl, HMe, 2Me, MeF, MeCl, MeBr calculated at MP2/aug-cc-pVDZ level of theory. For the sake of convenience, the different possible dimers formed by different combinations of the monomeric units will be labelled with respect to the R groups as R_1R_2, for instance dimer formed by combination of PA-2H and PA-BrCl will be labelled as 2H-BrCl. The solid symbols represent the shifts in the O–H/O–D stretching frequencies of acid due to change in the substituent on the dimerizing partner, while open symbols represent the shifts in the O–H/O–D stretching frequencies of the other phosphinic acids due to their dimerization with acid. The straight-lines are linear least-square fits to the data points and the slopes of these straight lines are called Stark tuning rates $(\Delta\vec{\mu})$.

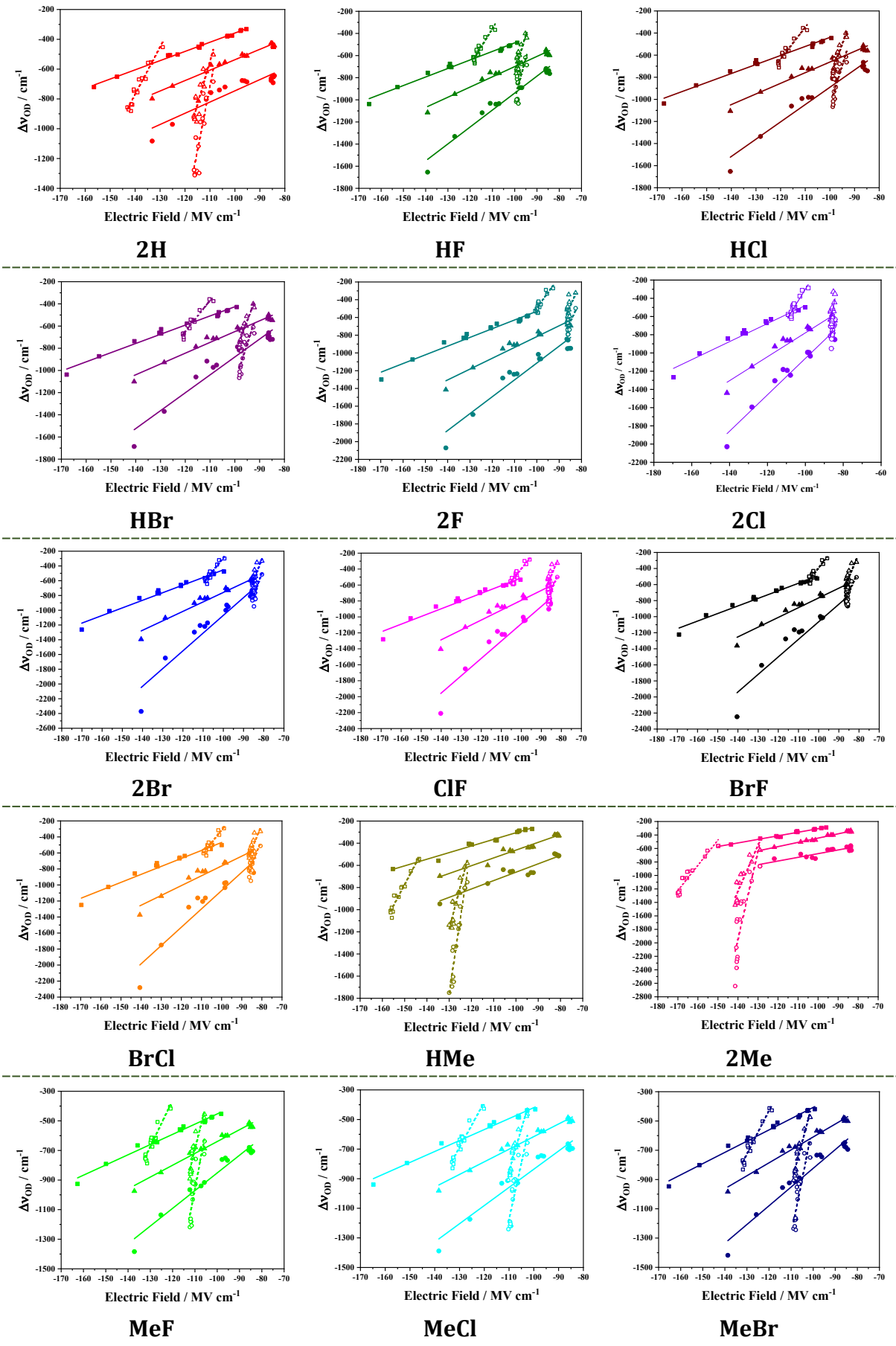

Figure S4. Plots of the red-shifts in the O–D stretching frequencies against the

corresponding Stark fields in the dimers of 2H, HF, HCl, HBr, 2F, 2Cl, 2Br, ClF, BrF, BrCl, HMe, 2Me, MeF, MeCl, MeBr. For the sake of convenience, the different possible dimers formed by different combinations of the monomeric units will be labelled with respect to the R groups as R_1R_2, i.e., dimer formed by combination of PA-2H and PA-BrCl will be labelled as (2H-BrCl). In each case the squares, circles and triangles represent harmonic MP2, harmonic B3LYP-D3, and anharmonic B3LYP-D3 frequency shifts calculated with aug/cc-pVDZ basis set, respectively. The solid symbols represent the shifts in the O–H/O–D stretching frequencies of acid due to change in the substituent on the dimerizing partner, while open symbols represent the shifts in the O–H/O–D stretching frequencies of the other phosphinic acids due to their dimerization with acid. The straight-lines are linear least-square fits to the data points and the slopes of these straight lines are called Stark tuning rates $(\Delta\vec{\mu})$.

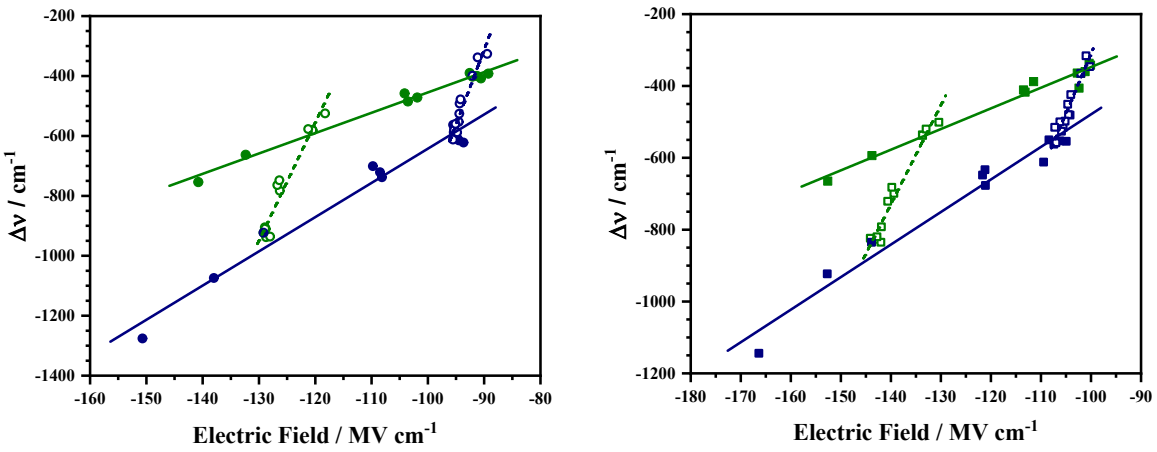

Figure S5. (Left) Plots of the red-shifts in the O–D stretching frequencies against the corresponding Stark fields in the dimers of parent phosphinic acid (2H, green circles) and ClF phosphinic acid (ClF, blue cirlces) calculated at B3LYP/PVTZ level of theory. (Right) Plots of the red-shifts in the O–D stretching frequencies against the corresponding Stark fields in the dimers of parent phosphinic acid (2H, green squares) and ClF phosphinic acid (ClF, blue squares) calculated at B2GP-PLYP/def2-TZVP/C level of theory. The solid symbols represent the shifts in the O–D stretching frequencies of acid due to change in the substituent on the dimerizing partner, while open symbols represent the shifts in the O–D stretching frequencies of the other phosphinic acids due to their dimerization with acid. The straight-lines are linear least-square fits to the data points and the slopes represent Stark tuning rates $(\Delta\vec{\mu})$.

Table S1. ZPE corrected dimerization energies (kJ mol^{-1}) and total electric field (MV cm^{-1}) (*in italics*) for various phosphinic acid dimers calculated at MP2/aug-cc-pVDZ level of theory. For the sake of convenience, the different possible dimers formed by different combinations of the monomeric units will be labelled with respect to the R groups as R_1R_2, i.e., dimer formed by combination of PA-2H and PA-BrCl will be labelled as (2H-BrCl).

	2H	**HF**	**HCl**	**HBr**	**2F**	**2Cl**	**2Br**	**ClF**	**BrF**	**BrCl**	**HMe**	**2Me**	**MeF**	**MeCl**	**MeBr**
2H	-83.6	-83.0	-83.7	-83.8	-85.0	-84.2	-83.7	-84.6	-84.3	-84.5	-86.7	-87.3	-84.2	-85.0	-84.3
	-267.3	***-252.3***	***-255.0***	***-254.7***	***-237.0***	***-244.0***	***-244.6***	***-240.1***	***-240.4***	***-244.3***	***-282.1***	***-285.4***	***-262.5***	***-263.3***	***-261.4***
HF		-79.5	-80.1	-80.2	-78.7	-78.4	-78.1	-78.8	-78.6	-78.2	-83.6	-89.8	-82.0	-82.8	-82.8
		-233.0	***-235.6***	***-235.4***	***-216.8***	***-223.8***	***-224.8***	***-220.0***	***-220.8***	***-224.5***	***-261.5***	***-275.8***	***-244.2***	***-245.6***	***-244.6***
HCl			-80.8	-81.0	-79.6	-79.2	-79.2	-79.7	-79.3	-79.1	-84.5	-90.8	-82.5	-83.6	-84.0
			-238.5	***-238.3***	***-220.1***	***-227.5***	***-228.1***	***-223.6***	***-224.5***	***-227.9***	***-263.5***	***-278.2***	***-246.6***	***-248.1***	***-247.5***
HBr				-81.2	-79.8	-79.7	-79.5	-80.0	-79.6	-80.0	-84.7	-91.0	-82.4	-84.0	-84.3
				-238.3	***-219.9***	***-227.0***	***-228.0***	***-223.4***	***-224.0***	***-227.6***	***-263.4***	***-278.1***	***-245.9***	***-248.0***	***-247.6***
2F					-75.4	-76.2	-76.1	-75.8	-75.9	-76.2	-87.5	-95.4	-83.5	-84.4	-84.5
					-199.2	***-207.4***	***-207.8***	***-204.3***	***-205.2***	***-207.5***	***-248.5***	***-265.7***	***-229.6***	***-232.2***	***-231.1***
2Cl						-77.0	-76.8	-76.6	-76.3	-77.2	-86.4	-94.0	-82.5	-83.7	-84.1
						-218.1	***-215.9***	***-211.0***	***-211.5***	***-215.5***	***-254.4***	***-271.3***	***-237.8***	***-239.0***	***-237.5***
2Br							-77.2	-76.5	-76.4	-76.8	-85.8	-93.6	-81.9	-83.5	-84.0
							-218.2	***-213.6***	***-213.6***	***-216.2***	***-255.8***	***-272.2***	***-237.8***	***-239.0***	***-238.5***
ClF								-76.5	-76.5	-76.7	-87.0	-94.9	-83.1	-84.2	-84.1
								-208.5	***-209.6***	***-214.4***	***-251.0***	***-267.4***	***-234.0***	***-235.1***	***-233.5***
BrF									-76.1	-76.7	-85.5	-93.2	-82.8	-83.8	-84.3
									-207.9	***-213.4***	***-251.5***	***-267.5***	***-234.7***	***-235.0***	***-233.9***
BrCl										-77.6	-86.5	-94.0	-82.5	-84.0	-84.5
										-215.8	***-255.1***	***-271.3***	***-237.6***	***-238.7***	***-238.3***
HMe											-84.0	-87.9	-84.7	-86.1	-86.2
											-288.0	***-298.7***	***-271.1***	***-271.8***	***-271.3***
2Me												-88.3	-89.0	-90.4	-90.7
												-299.6	***-283.5***	***-284.9***	***-284.0***
MeF													-83.7	-85.4	-85.5
													-255.3	***-257.2***	***-256.4***
MeCl														-85.7	-86.4
														-257.7	***-258.5***
MeBr															-86.3
															-256.7

Table S2. ZPE corrected dimerization energies (kJ mol^{-1}) and total electric field (MV cm-1) (*in italics*) for various phosphinic acid dimers calculated at B3LYP-D3/aug-cc-pVDZ level of theory. For the sake of convenience, the different possible dimers formed by different combinations of the monomeric units will be labelled with respect to the R groups as R_1R_2, i.e., dimer formed by combination of PA-2H and PA-BrCl will be labelled as (2H-BrCl).

	2H	**HF**	**HCl**	**HBr**	**2F**	**2Cl**	**2Br**	**ClF**	**BrF**	**BrCl**	**HMe**	**2Me**	**MeF**	**MeCl**	**MeBr**
2H	-89.1	-89.3	-89.8	-89.9	-92.2	-90.7	-89.9	-91.6	-91.3	-90.7	-92.6	-93.8	-90.5	-90.9	-91.1
	-223.0	***-211.7***	***-211.7***	***-210.9***	***-200.8***	***-200.8***	***-198.9***	***-201.6***	***-201.4***	***-200.5***	***-237.7***	***-241.8***	***-221.9***	***-219.2***	***-217.9***
HF		-86.9	-87.5	-87.4	-86.9	-86.2	-85.7	-86.6	-86.3	-85.8	-90.7	-97.4	-89.4	-90.0	-90.1
		-197.1	***-196.6***	***-195.8***	***-185.3***	***-184.4***	***-183.1***	***-185.1***	***-184.7***	***-183.1***	***-221.5***	***-234.3***	***-208.8***	***-206.8***	***-205.4***
HCl			-88.1	-88.1	-87.9	-86.9	-86.7	-87.3	-87.1	-86.9	-91.3	-98.0	-89.6	-90.4	-90.6
			-196.1	***-195.6***	***-185.3***	***-184.7***	***-183.1***	***-185.3***	***-185.0***	***-184.2***	***-221.4***	***-233.9***	***-207.7***	***-205.7***	***-204.1***
HBr				-88.3	-88.2	-87.2	-86.9	-87.9	-87.6	-87.3	-91.5	-98.1	-89.7	-90.5	-91.1
				-194.6	***-184.6***	***-184.0***	***-182.5***	***-184.7***	***-184.2***	***-183.6***	***-220.7***	***-233.2***	***-206.7***	***-204.7***	***-203.5***
2F					-83.9	-84.3	-84.1	-84.1	-84.1	-84.0	-95.7	-104.4	-91.8	-92.5	-92.7
					-172.1	***-172.2***	***-170.6***	***-172.6***	***-172.2***	***-170.8***	***-211.3***	***-226.5***	***-197.9***	***-196.4***	***-195.1***
2Cl						-84.4	-84.2	-84.6	-84.4	-84.6	-96.4	-103.3	-90.4	-91.1	-91.4
						-173.3	***-170.1***	***-171.6***	***-171.6***	***-171.2***	***-213.4***	***-225.7***	***-196.7***	***-195.2***	***-193.7***
2Br							-84.2	-84.4	-84.4	-83.9	-93.6	-102.3	-89.6	-90.4	-90.9
							-170.9	***-171.9***	***-171.7***	***-168.8***	***-209.6***	***-224.0***	***-195.6***	***-193.6***	***-192.2***
ClF								-84.6	-84.5	-84.3	-94.8	-103.4	-91.0	-91.9	-92.2
								-172.0	***-172.0***	***-172.5***	***-210.0***	***-225.0***	***-197.7***	***-195.9***	***-194.7***
BrF									-84.3	-84.5	-94.3	-102.8	-90.7	-91.6	-92.0
									-172.1	***-172.5***	***-209.5***	***-224.1***	***-197.2***	***-195.4***	***-193.9***
BrCl										-84.4	-94.3	-102.5	-90.0	-90.9	-91.3
										-171.1	***-210.7***	***-224.3***	***-196.6***	***-194.6***	***-193.2***
HMe											-90.9	-94.7	-91.6	-93.1	-94.0
											-245.9	***-256.1***	***-230.9***	***-228.4***	***-227.3***
2Me												-95.1	-96.1	-97.1	-97.3
												-258.0	***-243.0***	***-241.3***	***-240.0***
MeF													-91.0	-92.7	-92.8
													-219.8	***-217.8***	***-216.6***
MeCl														-92.3	-93.4
														-215.3	***-214.7***
MeBr															-92.9
															-212.6

Table S3. The harmonic vibrational frequencies (in cm^{-1}) of the donor O-H stretch along with its vibrational shift (in cm^{-1}) with respect to O-H stretch of the corresponding phosphinic acid monomer and the electric field (in MV cm^{-1}) along the bond calculated at MP2/aug-cc-pVDZ level of theory for the two cases namely, the effect on acid due to partner and the effect on partner due to acid respectively. For the sake of convenience, the different possible dimers formed by different combinations of the monomeric units will be labelled with respect to the R groups as R_1R_2, i.e., dimer formed by combination of PA-2H and PA-BrCl will be labelled as (2H-BrCl).

Dimer	ν_{O-H}	$\Delta\nu_{O-H}$	Field	ν_{O-H}	$\Delta\nu_{O-H}$	Field
	On PA-2H due to partner			On partner due to PA-2H		
2H-2H	3018	-772	-133.63	3018	-772	-133.64
2H-HF	3196	-593	-113.23	2731	-1055	-139.04
2H-HCl	3171	-618	-114.57	2730	-1040	-140.46
2H-HBr	3162	-627	-114.21	2742	-1026	-140.54
2H-2F	3348	-442	-95.39	2573	-1225	-141.63
2H-2Cl	3280	-510	-102.88	2587	-1166	-141.11
2H-2Br	3274	-515	-103.07	2580	-1160	-141.54
2H-ClF	3338	-451	-97.50	2568	-1209	-142.65
2H-BrF	3329	-461	-97.75	2582	-1191	-142.68
2H-BrCl	3284	-506	-101.16	2557	-1190	-143.11
2H-HMe	2885	-904	-147.23	3019	-773	-134.82
2H-2Me	2787	-1003	-156.48	3165	-625	-128.88
2H-MeF	3089	-701	-126.78	2862	-927	-135.71
2H-MeCl	3089	-700	-126.02	2856	-919	-137.25
2H-MeBr	3095	-695	-122.95	2842	-929	-138.50
	On PA-HF due to partner			On partner due to PA-HF		
HF-HF	2971	-815	-116.43	2964	-821	-116.56
HF-2H	2731	-1055	-139.04	3196	-593	-113.23
HF-HCl	2932	-854	-118.51	2996	-774	-117.10
HF-HBr	2923	-862	-118.24	3010	-758	-117.13
HF-2F	3118	-668	-98.84	2864	-934	-117.96
HF-2Cl	3040	-745	-105.75	2880	-874	-118.09
HF-2Br	3014	-772	-106.42	2881	-860	-118.35
HF-ClF	3083	-702	-102.03	2865	-912	-118.02
HF-BrF	3075	-710	-102.55	2880	-893	-118.28
HF-BrCl	3021	-764	-106.25	2864	-884	-118.30
HF-HMe	2552	-1234	-152.66	3297	-495	-108.80
HF-2Me	2298	-1488	-165.37	3286	-504	-110.46
HF-MeF	2847	-938	-129.09	3044	-744	-115.13
HF-MeCl	2807	-978	-129.52	3059	-716	-116.08
HF-MeBr	2803	-983	-128.42	3066	-705	-116.20
	On PA-HCl due to partner			On partner due to PA-HCl		
HCl-HCl	2953	-816	-119.26	2952	-818	-119.29
HCl-2H	2730	-1040	-140.46	3171	-618	-114.57
HCl-HF	2996	-774	-117.10	2932	-854	-118.51
HCl-HBr	2943	-827	-119.01	2966	-802	-119.33
HCl-2F	3157	-612	-99.41	2806	-992	-120.68

HCl-2Cl	3087	-682	-106.80	2846	-908	-120.74
HCl-2Br	3044	-726	-107.12	2827	-913	-121.02
HCl-ClF	3119	-651	-102.87	2818	-959	-120.74
HCl-BrF	3106	-664	-103.51	2835	-937	-121.02
HCl-BrCl	3076	-694	-107.07	2833	-915	-120.81
HCl-HMe	2553	-1217	-154.28	3287	-505	-109.26
HCl-2Me	2286	-1484	-167.32	3274	-516	-110.93
HCl-MeF	2873	-896	-129.90	3014	-774	-116.74
HCl-MeCl	2835	-935	-130.26	3028	-747	-117.83
HCl-MeBr	2825	-945	-129.43	3031	-740	-118.08
	On PA-HBr due to partner			On partner due to PA-HBr		
HBr-HBr	2952	-816	-119.16	2954	-814	-119.14
HBr-2H	2742	-1026	-140.54	3162	-627	-114.21
HBr-HF	3010	-758	-117.13	2923	-862	-118.24
HBr-HCl	2966	-802	-119.33	2943	-827	-119.01
HBr-2F	3179	-588	-99.23	2791	-1007	-120.64
HBr-2Cl	3113	-655	-106.46	2827	-927	-120.54
HBr-2Br	3063	-705	-107.03	2808	-933	-120.99
HBr-ClF	3139	-628	-102.77	2802	-975	-120.66
HBr-BrF	3130	-638	-103.21	2828	-945	-120.83
HBr-BrCl	3075	-693	-106.71	2819	-928	-120.92
HBr-HMe	2552	-1215	-154.77	3284	-508	-108.62
HBr-2Me	2285	-1482	-167.86	3270	-520	-110.24
HBr-MeF	2897	-871	-129.74	3008	-781	-116.20
HBr-MeCl	2849	-919	-130.44	3018	-756	-117.52
HBr-MeBr	2839	-929	-129.72	3021	-750	-117.85
	On PA-2F due to partner			On partner due to PA-2F		
2F-2F	3040	-758	-99.59	3040	-758	-99.59
2F-2H	2573	-1225	-141.63	3348	-442	-95.39
2F-HF	2864	-934	-117.96	3118	-668	-98.84
2F-HCl	2806	-992	-120.68	3157	-612	-99.41
2F-HBr	2791	-1007	-120.64	3179	-588	-99.23
2F-2Cl	2935	-864	-107.35	3062	-691	-100.06
2F-2Br	2903	-895	-108.04	3085	-656	-99.72
2F-ClF	2993	-805	-103.97	3038	-739	-100.37
2F-BrF	2982	-816	-104.42	3046	-727	-100.77
2F-BrCl	2918	-880	-107.59	3055	-692	-99.95
2F-HMe	2272	-1526	-155.74	3409	-383	-92.72
2F-2Me	1920	-1878	-169.73	3385	-405	-95.94
2F-MeF	2702	-1096	-131.44	3168	-621	-98.21
2F-MeCl	2642	-1156	-132.81	3186	-589	-99.42
2F-MeBr	2638	-1160	-131.82	3199	-572	-99.28
	On PA-2Cl due to partner			On partner due to PA-2Cl		
2Cl-2Cl	2956	-798	-109.08	2956	-798	-109.07
2Cl-2H	2587	-1166	-141.11	3280	-510	-102.88
2Cl-HF	2880	-874	-118.09	3040	-745	-105.75
2Cl-HCl	2846	-908	-120.74	3087	-682	-106.80
2Cl-HBr	2827	-927	-120.54	3113	-655	-106.46

2Cl-2F	3062	-691	-100.06	2935	-864	-107.35
2Cl-2Br	2926	-827	-108.36	2973	-768	-107.53
2Cl-ClF	3019	-735	-103.47	2946	-832	-107.49
2Cl-BrF	3014	-740	-104.06	2982	-791	-107.39
2Cl-BrCl	2941	-812	-108.01	2983	-764	-107.48
2Cl-HMe	2327	-1427	-155.95	3385	-407	-98.48
2Cl-2Me	1940	-1814	-169.70	3352	-438	-101.64
2Cl-MeF	2709	-1044	-132.31	3103	-685	-105.50
2Cl-MeCl	2658	-1095	-133.03	3107	-667	-105.98
2Cl-MeBr	2662	-1092	-131.55	3140	-632	-105.96
	On PA-2Br due to partner			On partner due to PA-2Br		
2Br-2Br	2960	-781	-109.10	2960	-781	-109.10
2Br-2H	2580	-1160	-141.54	3274	-515	-103.07
2Br-HF	2881	-860	-118.35	3014	-772	-106.42
2Br-HCl	2827	-913	-121.02	3044	-726	-107.12
2Br-HBr	2808	-933	-120.99	3063	-705	-107.03
2Br-2F	3085	-656	-99.72	2903	-895	-108.04
2Br-2Cl	2973	-768	-107.53	2926	-827	-108.36
2Br-ClF	3036	-704	-104.73	2934	-844	-108.88
2Br-BrF	3048	-693	-104.68	2961	-811	-108.89
2Br-BrCl	2960	-781	-107.86	2918	-830	-108.37
2Br-HMe	2308	-1433	-156.38	3367	-424	-99.44
2Br-2Me	1916	-1825	-170.10	3340	-450	-102.13
2Br-MeF	2727	-1014	-132.18	3086	-702	-105.58
2Br-MeCl	2682	-1059	-132.59	3110	-665	-106.44
2Br-MeBr	2666	-1075	-131.90	3119	-652	-106.60
	On PA-ClF due to partner			On partner due to PA-ClF		
ClF-ClF	2972	-805	-103.63	2987	-790	-104.88
ClF-2H	2568	-1209	-142.65	3338	-451	-97.50
ClF-HF	2865	-912	-118.02	3083	-702	-102.03
ClF-HCl	2818	-959	-120.74	3119	-651	-102.87
ClF-HBr	2802	-975	-120.66	3139	-628	-102.77
ClF-2F	3038	-739	-100.37	2993	-805	-103.97
ClF-2Cl	2946	-832	-107.49	3019	-735	-103.47
ClF-2Br	2934	-844	-108.88	3036	-704	-104.73
ClF-BrF	2961	-817	-104.14	2994	-779	-105.43
ClF-BrCl	2939	-838	-109.03	2985	-763	-105.40
ClF-HMe	2332	-1445	-155.26	3392	-399	-95.78
ClF-2Me	1931	-1846	-169.01	3372	-417	-98.39
ClF-MeF	2708	-1069	-131.73	3138	-651	-102.22
ClF-MeCl	2661	-1116	-132.44	3172	-602	-102.65
ClF-MeBr	2662	-1116	-131.13	3189	-583	-102.37
	On PA-BrF due to partner			On partner due to PA-BrF		
BrF-BrF	3028	-745	-103.99	3028	-744	-103.95
BrF-2H	2582	-1191	-142.68	3329	-461	-97.75
BrF-HF	2880	-893	-118.28	3075	-710	-102.55
BrF-HCl	2835	-937	-121.02	3106	-664	-103.51
BrF-HBr	2828	-945	-120.83	3130	-638	-103.21

BrF-2F	3046	-727	-100.77	2982	-816	-104.42
BrF-2Cl	2982	-791	-107.39	3014	-740	-104.06
BrF-2Br	2961	-811	-108.89	3048	-693	-104.68
BrF-ClF	2994	-779	-105.43	2961	-817	-104.14
BrF-BrCl	2977	-795	-108.70	3057	-690	-104.67
BrF-HMe	2379	-1394	-155.78	3399	-392	-95.77
BrF-2Me	2029	-1744	-169.15	3375	-414	-98.33
BrF-MeF	2721	-1052	-132.15	3132	-657	-102.54
BrF-MeCl	2697	-1076	-132.29	3173	-601	-102.71
BrF-MeBr	2678	-1095	-131.24	3181	-590	-102.64
	On PA-BrCl due to partner			On partner due to PA-BrCl		
BrCl-BrCl	2964	-783	-107.91	2965	-783	-107.90
BrCl-2H	2557	-1190	-143.11	3284	-506	-101.16
BrCl-HF	2864	-884	-118.30	3021	-764	-106.25
BrCl-HCl	2833	-915	-120.81	3076	-694	-107.07
BrCl-HBr	2819	-928	-120.92	3075	-693	-106.71
BrCl-2F	3055	-692	-99.95	2918	-880	-107.59
BrCl-2Cl	2983	-764	-107.48	2941	-812	-108.01
BrCl-2Br	2918	-830	-108.37	2960	-781	-107.86
BrCl-ClF	2985	-763	-105.40	2939	-838	-109.03
BrCl-BrF	3057	-690	-104.67	2977	-795	-108.70
BrCl-HMe	2296	-1451	-156.29	3378	-413	-98.78
BrCl-2Me	1959	-1789	-169.67	3347	-443	-101.64
BrCl-MeF	2738	-1010	-132.15	3097	-692	-105.41
BrCl-MeCl	2696	-1052	-132.49	3120	-654	-106.19
BrCl-MeBr	2678	-1069	-131.86	3127	-645	-106.43
	On PA-HMe due to partner			On partner due to PA-HMe		
HMe-HMe	3022	-770	-143.94	3019	-772	-144.05
HMe-2H	3019	-773	-134.82	2885	-904	-147.23
HMe-HF	3297	-495	-108.80	2552	-1234	-152.66
HMe-HCl	3287	-505	-109.26	2553	-1217	-154.28
HMe-HBr	3284	-508	-108.62	2552	-1215	-154.77
HMe-2F	3409	-383	-92.72	2272	-1526	-155.74
HMe-2Cl	3385	-407	-98.48	2327	-1427	-155.95
HMe-2Br	3367	-424	-99.44	2308	-1433	-156.38
HMe-ClF	3392	-399	-95.78	2332	-1445	-155.26
HMe-BrF	3399	-392	-95.77	2379	-1394	-155.78
HMe-BrCl	3378	-413	-98.78	2296	-1451	-156.29
HMe-2Me	2913	-879	-155.26	3040	-750	-143.49
HMe-MeF	3237	-554	-121.18	2685	-1104	-149.89
HMe-MeCl	3231	-561	-120.59	2667	-1108	-151.23
HMe-MeBr	3227	-565	-119.79	2655	-1117	-151.52
	On PA-2Me due to partner			On partner due to PA-2Me		
2Me-2Me	3011	-779	-149.82	3011	-779	-149.82
2Me-2H	3165	-625	-128.88	2787	-1003	-156.48
2Me-HF	3286	-504	-110.46	2298	-1488	-165.37
2Me-HCl	3274	-516	-110.93	2286	-1484	-167.32
2Me-HBr	3270	-520	-110.24	2285	-1482	-167.86

2Me-2F	3385	-405	-95.94	1920	-1878	-169.73
2Me-2Cl	3352	-438	-101.64	1940	-1814	-169.70
2Me-2Br	3340	-450	-102.13	1916	-1825	-170.10
2Me-ClF	3372	-417	-98.39	1931	-1846	-169.01
2Me-BrF	3375	-414	-98.33	2029	-1744	-169.15
2Me-BrCl	3347	-443	-101.64	1959	-1789	-169.67
2Me-HMe	3040	-750	-143.49	2913	-879	-155.26
2Me-MeF	3228	-562	-120.85	2499	-1289	-162.66
2Me-MeCl	3216	-574	-120.10	2469	-1306	-164.78
2Me-MeBr	3217	-573	-118.68	2457	-1314	-165.36
	On PA-MeF due to partner			On partner due to PA-MeF		
MeF-MeF	2933	-855	-127.65	2933	-855	-127.64
MeF-2H	2862	-927	-135.71	3089	-701	-126.78
MeF-HF	3044	-744	-115.13	2847	-938	-129.09
MeF-HCl	3014	-774	-116.74	2873	-896	-129.90
MeF-HBr	3008	-781	-116.20	2897	-871	-129.74
MeF-2F	3168	-621	-98.21	2702	-1096	-131.44
MeF-2Cl	3103	-685	-105.50	2709	-1044	-132.31
MeF-2Br	3086	-702	-105.58	2727	-1014	-132.18
MeF-ClF	3138	-651	-102.22	2708	-1069	-131.73
MeF-BrF	3132	-657	-102.54	2721	-1052	-132.15
MeF-BrCl	3097	-692	-105.41	2738	-1010	-132.15
MeF-HMe	2685	-1104	-149.89	3237	-554	-121.18
MeF-2Me	2499	-1289	-162.66	3228	-562	-120.85
MeF-MeCl	2896	-893	-128.03	2922	-852	-129.13
MeF-MeBr	2892	-897	-126.93	2921	-850	-129.51
	On PA-MeCl due to partner			On partner due to PA-MeCl		
MeCl-MeCl	2913	-861	-128.87	2913	-861	-128.87
MeCl-2H	2856	-919	-137.25	3089	-700	-126.02
MeCl-HF	3059	-716	-116.08	2807	-978	-129.52
MeCl-HCl	3028	-747	-117.83	2835	-935	-130.26
MeCl-HBr	3018	-756	-117.52	2849	-919	-130.44
MeCl-2F	3186	-589	-99.42	2642	-1156	-132.81
MeCl-2Cl	3107	-667	-105.98	2658	-1095	-133.03
MeCl-2Br	3110	-665	-106.44	2682	-1059	-132.59
MeCl-ClF	3172	-602	-102.65	2661	-1116	-132.44
MeCl-BrF	3173	-601	-102.71	2697	-1076	-132.29
MeCl-BrCl	3120	-654	-106.19	2696	-1052	-132.49
MeCl-HMe	2667	-1108	-151.23	3231	-561	-120.59
MeCl-2Me	2469	-1306	-164.78	3216	-574	-120.10
MeCl-MeF	2922	-852	-129.13	2896	-893	-128.03
MeCl-MeBr	2887	-887	-128.51	2889	-883	-129.96
	On PA-MeBr due to partner			On partner due to PA-MeBr		
MeBr-MeBr	2909	-863	-128.37	2909	-863	-128.37
MeBr-2H	2842	-929	-138.50	3095	-695	-122.95
MeBr-HF	3066	-705	-116.20	2803	-983	-128.42

MeBr-HCl	3031	-740	-118.08	2825	-945	-129.43
MeBr-HBr	3021	-750	-117.85	2839	-929	-129.72
MeBr-2F	3199	-572	-99.28	2638	-1160	-131.82
MeBr-2Cl	3140	-632	-105.96	2662	-1092	-131.55
MeBr-2Br	3119	-652	-106.60	2666	-1075	-131.90
MeBr-ClF	3189	-583	-102.37	2662	-1116	-131.13
MeBr-BrF	3181	-590	-102.64	2678	-1095	-131.24
MeBr-BrCl	3127	-645	-106.43	2678	-1069	-131.86
MeBr-HMe	2655	-1117	-151.52	3227	-565	-119.79
MeBr-2Me	2457	-1314	-165.36	3217	-573	-118.68
MeBr-MeF	2921	-850	-129.51	2892	-897	-126.93
MeBr-MeCl	2889	-883	-129.96	2887	-887	-128.51

Table S4. The harmonic vibrational frequencies (in cm^{-1}) of the donor O-D stretch along with its vibrational shift (in cm^{-1}) with respect to O-D stretch of the corresponding phosphinic acid monomer and the electric field (in MV cm^{-1}) along the bond calculated at MP2/aug-cc-pVDZ level of theory for the two cases namely, the effect on acid due to partner and the effect on partner due to acid respectively. For the sake of convenience, the different possible dimers formed by different combinations of the monomeric units will be labelled with respect to the R groups as R_1R_2, i.e., dimer formed by combination of PA-2H and PA-BrCl will be labelled as (2H-BrCl).

Dimer	$\nu_{O\text{-}D}$	$\Delta\nu_{O\text{-}D}$	Field	$\nu_{O\text{-}D}$	$\Delta\nu_{O\text{-}D}$	Field
	On PA-2H due to partner			On partner due to PA-2H		
2H-2H	2201	-557	-133.63	2201	-557	-133.64
2H-HF	2325	-433	-113.23	1999	-756	-139.04
2H-HCl	2308	-450	-114.57	1997	-747	-140.46
2H-HBr	2302	-456	-114.21	2005	-737	-140.54
2H-2F	2426	-332	-95.39	1883	-881	-141.63
2H-2Cl	2381	-377	-102.88	1892	-839	-141.11
2H-2Br	2378	-381	-103.07	1887	-835	-141.54
2H-ClF	2420	-338	-97.50	1879	-870	-142.65
2H-BrF	2415	-343	-97.75	1889	-856	-142.68
2H-BrCl	2383	-375	-101.16	1870	-857	-143.11
2H-HMe	2107	-651	-147.23	2202	-558	-134.82
2H-2Me	2038	-720	-156.48	2305	-453	-128.88
2H-MeF	2250	-508	-126.78	2091	-666	-135.71
2H-MeCl	2251	-507	-126.02	2086	-661	-137.25
2H-MeBr	2256	-502	-122.95	2076	-669	-138.50
	On PA-HF due to partner			On partner due to PA-HF		
HF-HF	2168	-587	-116.43	2163	-592	-116.56
HF-2H	1999	-756	-139.04	2325	-433	-113.23
HF-HCl	2141	-614	-118.51	2185	-559	-117.10
HF-HBr	2135	-620	-118.24	2195	-548	-117.13
HF-2F	2271	-484	-98.84	2093	-672	-117.96
HF-2Cl	2217	-539	-105.75	2101	-630	-118.09
HF-2Br	2198	-557	-106.42	2101	-621	-118.35

HF-ClF	2247	-508	-102.03	2093	-657	-118.02
HF-BrF	2241	-514	-102.55	2103	-643	-118.28
HF-BrCl	2203	-552	-106.25	2089	-638	-118.30
HF-HMe	1870	-885	-152.66	2391	-368	-108.80
HF-2Me	1717	-1038	-165.37	2414	-344	-110.46
HF-MeF	2081	-675	-129.09	2219	-538	-115.13
HF-MeCl	2053	-702	-129.52	2228	-519	-116.08
HF-MeBr	2050	-705	-128.42	2234	-511	-116.20
	On PA-HCl due to partner			On partner due to PA-HCl		
HCl-HCl	2155	-588	-119.26	2154	-589	-119.29
HCl-2H	1997	-747	-140.46	2308	-450	-114.57
HCl-HF	2185	-559	-117.10	2141	-614	-118.51
HCl-HBr	2148	-595	-119.01	2164	-578	-119.33
HCl-2F	2298	-446	-99.41	2053	-712	-120.68
HCl-2Cl	2249	-494	-106.80	2078	-654	-120.74
HCl-2Br	2218	-526	-107.12	2064	-658	-121.02
HCl-ClF	2271	-473	-102.87	2060	-689	-120.74
HCl-BrF	2262	-481	-103.51	2072	-674	-121.02
HCl-BrCl	2241	-503	-107.07	2068	-659	-120.81
HCl-HMe	1870	-873	-154.28	2386	-374	-109.26
HCl-2Me	1705	-1038	-167.32	2404	-354	-110.93
HCl-MeF	2098	-646	-129.90	2199	-558	-116.74
HCl-MeCl	2072	-672	-130.26	2207	-540	-117.83
HCl-MeBr	2064	-679	-129.43	2209	-535	-118.08
	On PA-HBr due to partner			On partner due to PA-HBr		
HBr-HBr	2154	-588	-119.16	2155	-587	-119.14
HBr-2H	2005	-737	-140.54	2302	-456	-114.21
HBr-HF	2195	-548	-117.13	2135	-620	-118.24
HBr-HCl	2164	-578	-119.33	2148	-595	-119.01
HBr-2F	2313	-429	-99.23	2043	-722	-120.64
HBr-2Cl	2267	-475	-106.46	2065	-667	-120.54
HBr-2Br	2232	-510	-107.03	2050	-672	-120.99
HBr-ClF	2285	-457	-102.77	2049	-700	-120.66
HBr-BrF	2279	-463	-103.21	2067	-679	-120.83
HBr-BrCl	2240	-502	-106.71	2059	-668	-120.92
HBr-HMe	1870	-872	-154.77	2384	-375	-108.62
HBr-2Me	1704	-1038	-167.86	2400	-357	-110.24
HBr-MeF	2114	-628	-129.74	2195	-562	-116.20
HBr-MeCl	2081	-661	-130.44	2201	-546	-117.52
HBr-MeBr	2074	-668	-129.72	2203	-542	-117.85
	On PA-2F due to partner			On partner due to PA-2F		
2F-2F	2218	-547	-99.59	2218	-547	-99.59
2F-2H	1883	-881	-141.63	2426	-332	-95.39
2F-HF	2093	-672	-117.96	2271	-484	-98.84
2F-HCl	2053	-712	-120.68	2298	-446	-99.41
2F-HBr	2043	-722	-120.64	2313	-429	-99.23
2F-2Cl	2143	-622	-107.35	2231	-501	-100.06
2F-2Br	2121	-644	-108.04	2246	-476	-99.72

2F-ClF	2184	-580	-103.97	2215	-534	-100.37
2F-BrF	2177	-588	-104.42	2221	-525	-100.77
2F-BrCl	2131	-634	-107.59	2225	-502	-99.95
2F-HMe	1691	-1074	-155.74	2488	-272	-92.72
2F-2Me	1465	-1299	-169.73	2468	-289	-95.94
2F-MeF	1977	-787	-131.44	2304	-453	-98.21
2F-MeCl	1935	-830	-132.81	2316	-431	-99.42
2F-MeBr	1933	-832	-131.82	2325	-419	-99.28
	On PA-2Cl due to partner			On partner due to PA-2Cl		
2Cl-2Cl	2155	-577	-109.08	2155	-576	-109.07
2Cl-2H	1892	-839	-141.11	2381	-377	-102.88
2Cl-HF	2101	-630	-118.09	2217	-539	-105.75
2Cl-HCl	2078	-654	-120.74	2249	-494	-106.80
2Cl-HBr	2065	-667	-120.54	2267	-475	-106.46
2Cl-2F	2231	-501	-100.06	2143	-622	-107.35
2Cl-2Br	2134	-597	-108.36	2167	-555	-107.53
2Cl-ClF	2200	-532	-103.47	2150	-599	-107.49
2Cl-BrF	2196	-535	-104.06	2175	-571	-107.39
2Cl-BrCl	2145	-586	-108.01	2174	-553	-107.48
2Cl-HMe	1724	-1007	-155.95	2473	-287	-98.48
2Cl-2Me	1468	-1263	-169.70	2445	-313	-101.64
2Cl-MeF	1980	-752	-132.31	2259	-498	-105.50
2Cl-MeCl	1944	-788	-133.03	2261	-486	-105.98
2Cl-MeBr	1947	-784	-131.55	2284	-461	-105.96
	On PA-2Br due to partner			On partner due to PA-2Br		
2Br-2Br	2157	-564	-109.10	2157	-564	-109.10
2Br-2H	1887	-835	-141.54	2378	-381	-103.07
2Br-HF	2101	-621	-118.35	2198	-557	-106.42
2Br-HCl	2064	-658	-121.02	2218	-526	-107.12
2Br-HBr	2050	-672	-120.99	2232	-510	-107.03
2Br-2F	2246	-476	-99.72	2121	-644	-108.04
2Br-2Cl	2167	-555	-107.53	2134	-597	-108.36
2Br-ClF	2212	-510	-104.73	2142	-608	-108.88
2Br-BrF	2220	-502	-104.68	2161	-584	-108.89
2Br-BrCl	2157	-565	-107.86	2128	-599	-108.37
2Br-HMe	1710	-1012	-156.38	2460	-299	-99.44
2Br-2Me	1459	-1263	-170.10	2437	-321	-102.13
2Br-MeF	1991	-730	-132.18	2248	-509	-105.58
2Br-MeCl	1960	-762	-132.59	2264	-483	-106.44
2Br-MeBr	1949	-773	-131.90	2270	-475	-106.60
	On PA-ClF due to partner			On partner due to PA-ClF		
ClF-ClF	2168	-581	-103.63	2179	-570	-104.88
ClF-2H	1879	-870	-142.65	2420	-338	-97.50
ClF-HF	2093	-657	-118.02	2247	-508	-102.03
ClF-HCl	2060	-689	-120.74	2271	-473	-102.87
ClF-HBr	2049	-700	-120.66	2285	-457	-102.77
ClF-2F	2215	-534	-100.37	2184	-580	-103.97
ClF-2Cl	2150	-599	-107.49	2200	-532	-103.47

ClF-2Br	2142	-608	-108.88	2212	-510	-104.73
ClF-BrF	2160	-590	-104.14	2183	-562	-105.43
ClF-BrCl	2145	-604	-109.03	2175	-552	-105.40
ClF-HMe	1731	-1018	-155.26	2479	-281	-95.78
ClF-2Me	1468	-1281	-169.01	2460	-298	-98.39
ClF-MeF	1981	-768	-131.73	2283	-473	-102.22
ClF-MeCl	1948	-801	-132.44	2307	-440	-102.65
ClF-MeBr	1949	-800	-131.13	2319	-426	-102.37
	On PA-BrF due to partner			On partner due to PA-BrF		
BrF-BrF	2208	-538	-103.99	2208	-537	-103.95
BrF-2H	1889	-856	-142.68	2415	-343	-97.75
BrF-HF	2103	-643	-118.28	2241	-514	-102.55
BrF-HCl	2072	-674	-121.02	2262	-481	-103.51
BrF-HBr	2067	-679	-120.83	2279	-463	-103.21
BrF-2F	2221	-525	-100.77	2177	-588	-104.42
BrF-2Cl	2175	-571	-107.39	2196	-535	-104.06
BrF-2Br	2161	-584	-108.89	2220	-502	-104.68
BrF-ClF	2183	-562	-105.43	2160	-590	-104.14
BrF-BrCl	2173	-573	-108.70	2227	-500	-104.67
BrF-HMe	1764	-981	-155.78	2486	-273	-95.77
BrF-2Me	1523	-1223	-169.15	2462	-296	-98.33
BrF-MeF	1990	-756	-132.15	2280	-477	-102.54
BrF-MeCl	1974	-772	-132.29	2309	-438	-102.71
BrF-MeBr	1961	-785	-131.24	2314	-430	-102.64
	On PA-BrCl due to partner			On partner due to PA-BrCl		
BrCl-BrCl	2161	-566	-107.91	2161	-565	-107.90
BrCl-2H	1870	-857	-143.11	2383	-375	-101.16
BrCl-HF	2089	-638	-118.30	2203	-552	-106.25
BrCl-HCl	2068	-659	-120.81	2241	-503	-107.07
BrCl-HBr	2059	-668	-120.92	2240	-502	-106.71
BrCl-2F	2225	-502	-99.95	2131	-634	-107.59
BrCl-2Cl	2174	-553	-107.48	2145	-586	-108.01
BrCl-2Br	2128	-599	-108.37	2157	-565	-107.86
BrCl-ClF	2175	-552	-105.40	2145	-604	-109.03
BrCl-BrF	2227	-500	-104.67	2173	-573	-108.70
BrCl-HMe	1702	-1025	-156.29	2467	-292	-98.78
BrCl-2Me	1477	-1250	-169.67	2442	-316	-101.64
BrCl-MeF	2000	-727	-132.15	2256	-501	-105.41
BrCl-MeCl	1971	-756	-132.49	2271	-475	-106.19
BrCl-MeBr	1959	-768	-131.86	2276	-469	-106.43
	On PA-HMe due to partner			On partner due to PA-HMe		
HMe-HMe	2204	-556	-143.94	2202	-557	-144.05
HMe-2H	2202	-558	-134.82	2107	-651	-147.23
HMe-HF	2391	-368	-108.80	1870	-885	-152.66
HMe-HCl	2386	-374	-109.26	1870	-873	-154.28
HMe-HBr	2384	-375	-108.62	1870	-872	-154.77
HMe-2F	2488	-272	-92.72	1691	-1074	-155.74
HMe-2Cl	2473	-287	-98.48	1724	-1007	-155.95

HMe-2Br	2460	-299	-99.44	1710	-1012	-156.38
HMe-ClF	2479	-281	-95.78	1731	-1018	-155.26
HMe-BrF	2486	-273	-95.77	1764	-981	-155.78
HMe-BrCl	2467	-292	-98.78	1702	-1025	-156.29
HMe-2Me	2126	-633	-155.26	2217	-541	-143.49
HMe-MeF	2354	-405	-121.18	1966	-791	-149.89
HMe-MeCl	2350	-409	-120.59	1952	-795	-151.23
HMe-MeBr	2347	-413	-119.79	1943	-801	-151.52
	On PA-2Me due to partner			On partner due to PA-2Me		
2Me-2Me	2196	-562	-149.82	2196	-562	-149.82
2Me-2H	2305	-453	-128.88	2038	-720	-156.48
2Me-HF	2414	-344	-110.46	1717	-1038	-165.37
2Me-HCl	2404	-354	-110.93	1705	-1038	-167.32
2Me-HBr	2400	-357	-110.24	1704	-1038	-167.86
2Me-2F	2468	-289	-95.94	1465	-1299	-169.73
2Me-2Cl	2445	-313	-101.64	1468	-1263	-169.70
2Me-2Br	2437	-321	-102.13	1459	-1263	-170.10
2Me-ClF	2460	-298	-98.39	1468	-1281	-169.01
2Me-BrF	2462	-296	-98.33	1523	-1223	-169.15
2Me-BrCl	2442	-316	-101.64	1477	-1250	-169.67
2Me-HMe	2217	-541	-143.49	2126	-633	-155.26
2Me-MeF	2341	-417	-120.85	1831	-926	-162.66
2Me-MeCl	2331	-427	-120.10	1807	-940	-164.78
2Me-MeBr	2330	-428	-118.68	1798	-947	-165.36
	On PA-MeF due to partner			On partner due to PA-MeF		
MeF-MeF	2141	-616	-127.65	2141	-616	-127.64
MeF-2H	2091	-666	-135.71	2250	-508	-126.78
MeF-HF	2219	-538	-115.13	2081	-675	-129.09
MeF-HCl	2199	-558	-116.74	2098	-646	-129.90
MeF-HBr	2195	-562	-116.20	2114	-628	-129.74
MeF-2F	2304	-453	-98.21	1977	-787	-131.44
MeF-2Cl	2259	-498	-105.50	1980	-752	-132.31
MeF-2Br	2248	-509	-105.58	1991	-730	-132.18
MeF-ClF	2283	-473	-102.22	1981	-768	-131.73
MeF-BrF	2280	-477	-102.54	1990	-756	-132.15
MeF-BrCl	2256	-501	-105.41	2000	-727	-132.15
MeF-HMe	1965	-791	-149.89	2354	-405	-121.18
MeF-2Me	1831	-926	-162.66	2341	-417	-120.85
MeF-MeCl	2114	-643	-128.03	2132	-615	-129.13
MeF-MeBr	2112	-645	-126.93	2131	-614	-129.51
	On PA-MeCl due to partner			On partner due to PA-MeCl		
MeCl-MeCl	2126	-621	-128.87	2126	-621	-128.87
MeCl-2H	2086	-661	-137.25	2251	-507	-126.02
MeCl-HF	2228	-519	-116.08	2053	-702	-129.52
MeCl-HCl	2207	-540	-117.83	2072	-672	-130.26
MeCl-HBr	2201	-546	-117.52	2081	-661	-130.44
MeCl-2F	2316	-431	-99.42	1935	-830	-132.81
MeCl-2Cl	2261	-486	-105.98	1944	-788	-133.03

MeCl-2Br	2264	-483	-106.44	1960	-762	-132.59
MeCl-ClF	2307	-440	-102.65	1948	-801	-132.44
MeCl-BrF	2309	-438	-102.71	1974	-772	-132.29
MeCl-BrCl	2271	-475	-106.19	1971	-756	-132.49
MeCl-HMe	1952	-795	-151.23	2350	-409	-120.59
MeCl-2Me	1807	-940	-164.78	2331	-427	-120.10
MeCl-MeF	2132	-615	-129.13	2114	-643	-128.03
MeCl-MeBr	2108	-639	-128.51	2108	-636	-129.96
	On PA-MeBr due to partner			On partner due to PA-MeBr		
MeBr-MeBr	2123	-622	-128.37	2123	-622	-128.37
MeBr-2H	2076	-669	-138.50	2256	-502	-122.95
MeBr-HF	2234	-511	-116.20	2050	-705	-128.42
MeBr-HCl	2209	-535	-118.08	2064	-679	-129.43
MeBr-HBr	2203	-542	-117.85	2074	-668	-129.72
MeBr-2F	2325	-419	-99.28	1933	-832	-131.82
MeBr-2Cl	2284	-461	-105.96	1947	-784	-131.55
MeBr-2Br	2270	-475	-106.60	1949	-773	-131.90
MeBr-ClF	2319	-426	-102.37	1949	-800	-131.13
MeBr-BrF	2314	-430	-102.64	1961	-785	-131.24
MeBr-BrCl	2276	-469	-106.43	1959	-768	-131.86
MeBr-HMe	1943	-801	-151.52	2347	-413	-119.79
MeBr-2Me	1798	-947	-165.36	2330	-428	-118.68
MeBr-MeF	2131	-614	-129.51	2112	-645	-126.93
MeBr-MeCl	2108	-636	-129.96	2108	-639	-128.51

Table S5. The harmonic vibrational frequencies (in cm^{-1}) of the donor O-D stretch along with its vibrational shift (in cm^{-1}) with respect to O-D stretch of the corresponding phosphinic acid monomer and the electric field (in MV cm^{-1}) along the bond calculated at B3LYP-D3/aug-cc-pVDZ level of theory for the two cases namely, the effect on acid due to partner and the effect on partner due to acid respectively. For the sake of convenience, the different possible dimers formed by different combinations of the monomeric units will be labelled with respect to the R groups as R_1R_2, i.e., dimer formed by combination of PA-2H and PA-BrCl will be labelled as (2H-BrCl).

Dimer	$\nu_{O\text{-}D}$	$\Delta\nu_{O\text{-}D}$	Field	$\nu_{O\text{-}D}$	$\Delta\nu_{O\text{-}D}$	Field
	On PA-2H due to partner			On partner due to PA-2H		
2H-2H	2144	-615	-111.49	2144	-615	-111.49
2H-HF	2258	-501	-97.07	1941	-814	-114.63
2H-HCl	2248	-511	-96.11	1955	-794	-115.58
2H-HBr	2248	-512	-95.21	1963	-786	-115.70
2H-2F	2333	-426	-85.48	1811	-954	-115.31
2H-2Cl	2315	-444	-84.68	1809	-930	-116.11
2H-2Br	2306	-453	-84.57	1828	-903	-114.34
2H-ClF	2331	-428	-85.45	1816	-936	-116.10
2H-BrF	2331	-428	-85.01	1830	-920	-116.37

2H-BrCl	2317	-442	-84.19	1825	-911	-116.34
2H-HMe	2045	-714	-125.06	2166	-600	-112.69
2H-2Me	1960	-799	-133.17	2264	-504	-108.68
2H-MeF	2187	-572	-109.65	2043	-718	-112.29
2H-MeCl	2191	-568	-106.21	2054	-702	-112.95
2H-MeBr	2205	-554	-103.98	2051	-705	-113.88
	On PA-HF due to partner			On partner due to PA-HF		
HF-HF	2099	-656	-98.58	2100	-655	-98.56
HF-2H	1941	-814	-114.63	2258	-501	-97.07
HF-HCl	2085	-670	-97.62	2124	-625	-98.94
HF-HBr	2086	-668	-96.82	2135	-613	-98.93
HF-2F	2207	-548	-85.90	2004	-761	-99.35
HF-2Cl	2165	-590	-85.61	2024	-715	-98.80
HF-2Br	2157	-597	-84.31	2032	-699	-98.75
HF-ClF	2188	-567	-86.03	2021	-732	-99.03
HF-BrF	2184	-570	-85.57	2033	-717	-99.14
HF-BrCl	2163	-592	-84.74	2014	-722	-98.35
HF-HMe	1807	-948	-126.95	2326	-440	-94.58
HF-2Me	1639	-1115	-139.13	2367	-400	-95.20
HF-MeF	2003	-752	-110.99	2165	-597	-97.83
HF-MeCl	1992	-763	-108.46	2184	-573	-98.30
HF-MeBr	1996	-759	-107.06	2189	-567	-98.36
	On PA-HCl due to partner			On partner due to PA-HCl		
HCl-HCl	2109	-640	-98.06	2110	-639	-98.05
HCl-2H	1955	-794	-115.58	2248	-511	-96.11
HCl-HF	2124	-625	-98.94	2085	-670	-97.62
HCl-HBr	2106	-643	-97.38	2116	-633	-98.23
HCl-2F	2237	-512	-86.43	1977	-788	-98.84
HCl-2Cl	2201	-548	-86.63	2006	-733	-98.04
HCl-2Br	2189	-559	-84.77	2006	-725	-98.33
HCl-ClF	2218	-531	-86.61	1992	-760	-98.67
HCl-BrF	2216	-533	-86.31	2006	-744	-98.72
HCl-BrCl	2191	-558	-85.70	2015	-720	-98.51
HCl-HMe	1816	-933	-128.16	2329	-437	-93.21
HCl-2Me	1643	-1106	-140.41	2367	-400	-93.53
HCl-MeF	2032	-717	-111.34	2160	-601	-96.32
HCl-MeCl	2024	-725	-108.70	2174	-582	-96.96
HCl-MeBr	2025	-724	-107.26	2185	-571	-96.87
	On PA-HBr due to partner			On partner due to PA-HBr		
HBr-HBr	2119	-629	-97.30	2119	-629	-97.29
HBr-2H	1963	-786	-115.70	2248	-512	-95.21
HBr-HF	2135	-613	-98.93	2086	-668	-96.82
HBr-HCl	2116	-633	-98.23	2106	-643	-97.38
HBr-2F	2251	-498	-86.36	1970	-794	-98.24
HBr-2Cl	2215	-533	-86.60	1998	-741	-97.41
HBr-2Br	2201	-547	-84.86	2002	-729	-97.61
HBr-ClF	2230	-519	-86.68	1985	-767	-98.06
HBr-BrF	2230	-519	-86.19	2007	-743	-98.05

HBr-BrCl	2206	-543	-85.74	2010	-725	-97.81
HBr-HMe	1821	-927	-128.50	2333	-433	-92.17
HBr-2Me	1647	-1101	-140.63	2206	-562	-92.57
HBr-MeF	2046	-702	-111.29	2162	-600	-95.41
HBr-MeCl	2037	-712	-108.73	2177	-580	-96.00
HBr-MeBr	2038	-711	-107.37	2179	-577	-96.15
	On PA-2F due to partner			On partner due to PA-2F		
2F-2F	2142	-623	-86.03	2142	-622	-86.04
2F-2H	1811	-954	-115.31	2333	-426	-85.48
2F-HF	2004	-761	-99.35	2207	-548	-85.90
2F-HCl	1977	-788	-98.84	2237	-512	-86.43
2F-HBr	1970	-794	-98.24	2251	-498	-86.36
2F-2Cl	2083	-681	-86.27	2159	-580	-85.90
2F-2Br	2071	-693	-84.84	2172	-560	-85.78
2F-ClF	2112	-653	-86.54	2153	-600	-86.07
2F-BrF	2107	-657	-86.03	2164	-587	-86.21
2F-BrCl	2078	-686	-85.44	2150	-585	-85.34
2F-HMe	1599	-1165	-128.69	2443	-323	-82.63
2F-2Me	1350	-1415	-140.80	2426	-342	-85.70
2F-MeF	1873	-891	-112.25	2249	-512	-85.62
2F-MeCl	1855	-910	-110.25	2270	-487	-86.19
2F-MeBr	1859	-905	-108.89	2278	-478	-86.17
	On PA-2Cl due to partner			On partner due to PA-2Cl		
2Cl-2Cl	2104	-635	-86.67	2104	-635	-86.67
2Cl-2H	1809	-930	-116.11	2315	-444	-84.68
2Cl-HF	2024	-715	-98.80	2165	-590	-85.61
2Cl-HCl	2006	-733	-98.04	2201	-548	-86.63
2Cl-HBr	1998	-741	-97.41	2215	-533	-86.60
2Cl-2F	2159	-580	-85.90	2083	-681	-86.27
2Cl-2Br	2095	-644	-84.46	2121	-610	-85.66
2Cl-ClF	2137	-602	-85.77	2100	-652	-85.86
2Cl-BrF	2130	-609	-85.49	2115	-635	-86.09
2Cl-BrCl	2100	-639	-85.39	2127	-608	-85.85
2Cl-HMe	1590	-1149	-128.20	2437	-328	-85.20
2Cl-2Me	1300	-1439	-141.38	2415	-353	-84.33
2Cl-MeF	1891	-848	-111.71	2219	-543	-85.01
2Cl-MeCl	1874	-865	-109.60	2238	-518	-85.59
2Cl-MeBr	1879	-860	-107.90	2256	-500	-85.78
	On PA-2Br due to partner			On partner due to PA-2Br		
2Br-2Br	2106	-625	-85.43	2106	-626	-85.43
2Br-2H	1828	-903	-114.34	2306	-453	-84.57
2Br-HF	2032	-699	-98.75	2157	-597	-84.31
2Br-HCl	2006	-725	-98.33	2189	-559	-84.77
2Br-HBr	2002	-729	-97.61	2201	-547	-84.86
2Br-2F	2172	-560	-85.78	2071	-693	-84.84
2Br-2Cl	2121	-610	-85.66	2095	-644	-84.46
2Br-ClF	2137	-594	-86.60	2087	-665	-85.34
2Br-BrF	2138	-593	-86.03	2109	-641	-85.62

2Br-BrCl	2118	-614	-84.76	2086	-650	-84.09
2Br-HMe	1628	-1103	-128.71	2433	-333	-80.89
2Br-2Me	1337	-1394	-140.69	2414	-353	-83.35
2Br-MeF	1895	-836	-111.50	2219	-542	-84.06
2Br-MeCl	1891	-840	-109.19	2245	-511	-84.40
2Br-MeBr	1897	-834	-107.83	2255	-501	-84.33
	On PA-ClF due to partner			On partner due to PA-ClF		
ClF-ClF	2124	-629	-86.22	2119	-633	-85.81
ClF-2H	1816	-936	-116.10	2331	-428	-85.45
ClF-HF	2021	-732	-99.03	2188	-567	-86.03
ClF-HCl	1992	-760	-98.67	2218	-531	-86.61
ClF-HBr	1985	-767	-98.06	2230	-519	-86.68
ClF-2F	2153	-600	-86.07	2112	-653	-86.54
ClF-2Cl	2100	-652	-85.86	2137	-602	-85.77
ClF-2Br	2087	-665	-85.34	2137	-594	-86.60
ClF-BrF	2117	-636	-85.44	2142	-608	-86.59
ClF-BrCl	2089	-663	-86.27	2120	-616	-86.25
ClF-HMe	1624	-1128	-127.96	2178	-588	-82.03
ClF-2Me	1349	-1404	-140.22	2426	-341	-84.74
ClF-MeF	1893	-860	-111.91	2237	-525	-85.84
ClF-MeCl	1874	-878	-109.63	2258	-498	-86.31
ClF-MeBr	1878	-875	-108.34	2267	-490	-86.35
	On PA-BrF due to partner			On partner due to PA-BrF		
BrF-BrF	2141	-610	-85.99	2142	-609	-86.07
BrF-2H	1830	-920	-116.37	2331	-428	-85.01
BrF-HF	2033	-717	-99.14	2184	-570	-85.57
BrF-HCl	2006	-744	-98.72	2216	-533	-86.31
BrF-HBr	2007	-743	-98.05	2230	-519	-86.19
BrF-2F	2164	-587	-86.21	2107	-657	-86.03
BrF-2Cl	2115	-635	-86.09	2130	-609	-85.49
BrF-2Br	2109	-641	-85.62	2138	-593	-86.03
BrF-ClF	2142	-608	-86.59	2117	-636	-85.44
BrF-BrCl	2116	-635	-86.26	2146	-590	-86.22
BrF-HMe	1656	-1094	-128.25	2445	-321	-81.24
BrF-2Me	1388	-1362	-140.43	2433	-335	-83.69
BrF-MeF	1907	-843	-112.05	2238	-523	-85.16
BrF-MeCl	1898	-852	-109.68	2260	-497	-85.72
BrF-MeBr	1908	-842	-108.30	2275	-482	-85.65
	On PA-BrCl due to partner			On partner due to PA-BrCl		
BrCl-BrCl	2119	-617	-85.57	2119	-616	-85.58
BrCl-2H	1825	-911	-116.34	2317	-442	-84.19
BrCl-HF	2014	-722	-98.35	2163	-592	-84.74
BrCl-HCl	2015	-720	-98.51	2191	-558	-85.70
BrCl-HBr	2010	-725	-97.81	2206	-543	-85.74
BrCl-2F	2150	-585	-85.34	2078	-686	-85.44
BrCl-2Cl	2127	-608	-85.85	2100	-639	-85.39
BrCl-2Br	2086	-650	-84.09	2118	-614	-84.76
BrCl-ClF	2120	-616	-86.25	2089	-663	-86.27

BrCl-BrF	2146	-590	-86.22	2116	-635	-86.26
BrCl-HMe	1597	-1139	-130.00	2435	-331	-80.69
BrCl-2Me	1363	-1373	-140.61	2418	-349	-83.70
BrCl-MeF	1914	-822	-111.88	2223	-539	-84.76
BrCl-MeCl	1904	-831	-109.42	2247	-509	-85.17
BrCl-MeBr	1909	-827	-108.06	2257	-500	-85.15
	On PA-HMe due to partner			On partner due to PA-HMe		
HMe-HMe	2152	-614	-122.97	2152	-614	-122.96
HMe-2H	2166	-600	-112.69	2045	-714	-125.06
HMe-HF	2326	-440	-94.58	1807	-948	-126.95
HMe-HCl	2329	-437	-93.21	1816	-933	-128.16
HMe-HBr	2333	-433	-92.17	1821	-927	-128.50
HMe-2F	2443	-323	-82.63	1599	-1165	-128.69
HMe-2Cl	2437	-328	-85.20	1590	-1149	-128.20
HMe-2Br	2433	-333	-80.89	1628	-1103	-128.71
HMe-ClF	2440	-326	-82.03	1624	-1128	-127.96
HMe-BrF	2445	-321	-81.24	1656	-1094	-128.25
HMe-BrCl	2435	-331	-80.69	1597	-1139	-130.00
HMe-2Me	2069	-697	-134.20	2187	-580	-121.87
HMe-MeF	2310	-456	-105.70	1913	-848	-125.25
HMe-MeCl	2302	-464	-102.61	1912	-844	-125.81
HMe-MeBr	2292	-474	-101.54	1907	-849	-125.76
	On PA-2Me due to partner			On partner due to PA-2Me		
2Me-2Me	2142	-625	-129.01	2142	-625	-129.00
2Me-2H	2264	-504	-108.68	1960	-799	-133.17
2Me-HF	2367	-400	-95.20	1639	-1115	-139.13
2Me-HCl	2367	-400	-93.53	1643	-1106	-140.41
2Me-HBr	2368	-400	-92.57	1647	-1101	-140.63
2Me-2F	2426	-342	-85.70	1350	-1415	-140.80
2Me-2Cl	2415	-353	-84.33	1300	-1439	-141.38
2Me-2Br	2414	-353	-83.35	1337	-1394	-140.69
2Me-ClF	2426	-341	-84.74	1349	-1404	-140.22
2Me-BrF	2433	-335	-83.69	1388	-1362	-140.43
2Me-BrCl	2418	-349	-83.70	1363	-1373	-140.61
2Me-HMe	2187	-580	-121.87	2069	-697	-134.20
2Me-MeF	2289	-479	-105.85	1787	-975	-137.17
2Me-MeCl	2290	-478	-102.93	1775	-981	-138.35
2Me-MeBr	2292	-475	-101.35	1772	-984	-138.65
	On PA-MeF due to partner			On partner due to PA-MeF		
MeF-MeF	2083	-678	-109.91	2083	-679	-109.91
MeF-2H	2043	-718	-112.29	2187	-572	-109.65
MeF-HF	2165	-597	-97.83	2003	-752	-110.99
MeF-HCl	2160	-601	-96.32	2032	-717	-111.34
MeF-HBr	2162	-600	-95.41	2046	-702	-111.29
MeF-2F	2249	-512	-85.62	1873	-891	-112.25
MeF-2Cl	2219	-543	-85.01	1891	-848	-111.71
MeF-2Br	2219	-542	-84.06	1895	-836	-111.50
MeF-ClF	2237	-525	-85.84	1893	-860	-111.91

MeF-BrF	2238	-523	-85.16	1907	-843	-112.05
MeF-BrCl	2223	-539	-84.76	1914	-822	-111.88
MeF-HMe	1913	-848	-125.25	2310	-456	-105.70
MeF-2Me	1787	-975	-137.17	2289	-479	-105.85
MeF-MeCl	2072	-689	-107.26	2086	-671	-110.55
MeF-MeBr	2074	-687	-105.76	2083	-674	-110.81
	On PA-MeCl due to partner			On partner due to PA-MeCl		
MeCl-MeCl	2095	-662	-107.63	2095	-662	-107.62
MeCl-2H	2054	-702	-112.95	2191	-568	-106.21
MeCl-HF	2184	-573	-98.30	1992	-763	-108.46
MeCl-HCl	2174	-582	-96.96	2024	-725	-108.70
MeCl-HBr	2177	-580	-96.00	2037	-712	-108.73
MeCl-2F	2270	-487	-86.19	1855	-910	-110.25
MeCl-2Cl	2238	-518	-85.59	1874	-865	-109.60
MeCl-2Br	2245	-511	-84.40	1891	-840	-109.19
MeCl-ClF	2258	-498	-86.31	1874	-878	-109.63
MeCl-BrF	2260	-497	-85.72	1898	-852	-109.68
MeCl-BrCl	2247	-509	-85.17	1904	-831	-109.42
MeCl-HMe	1912	-844	-125.81	2302	-464	-102.61
MeCl-2Me	1775	-981	-138.35	2290	-478	-102.93
MeCl-MeF	2086	-671	-110.55	2072	-689	-107.26
MeCl-MeBr	2082	-675	-106.53	2079	-678	-108.18
	On PA-MeBr due to partner			On partner due to PA-MeBr		
MeBr-MeBr	2100	-656	-106.28	2101	-656	-106.30
MeBr-2H	2051	-705	-113.88	2205	-554	-103.98
MeBr-HF	2189	-567	-98.36	1996	-759	-107.06
MeBr-HCl	2185	-571	-96.87	2025	-724	-107.26
MeBr-HBr	2179	-577	-96.15	2038	-711	-107.37
MeBr-2F	2278	-478	-86.17	1859	-905	-108.89
MeBr-2Cl	2256	-500	-85.78	1879	-860	-107.90
MeBr-2Br	2255	-501	-84.33	1897	-834	-107.83
MeBr-ClF	2267	-490	-86.35	1878	-875	-108.34
MeBr-BrF	2275	-482	-85.65	1908	-842	-108.30
MeBr-BrCl	2257	-500	-85.15	1909	-827	-108.06
MeBr-HMe	1907	-849	-125.76	2292	-474	-101.54
MeBr-2Me	1772	-984	-138.65	2292	-475	-101.35
MeBr-MeF	2083	-674	-110.81	2074	-687	-105.76
MeBr-MeCl	2079	-678	-108.18	2082	-675	-106.53

Table S6. The anharmonic vibrational frequencies (in cm^{-1}) of the donor O-D stretch along with its vibrational shift (in cm^{-1}) with respect to O-D stretch of the corresponding phosphinic acid monomer and the electric field (in MV cm^{-1}) along the bond calculated at B3LYP-D3/aug-cc-pVDZ level of theory using VPT2 method for the two cases namely, the effect on acid due to partner and the effect on partner due to acid respectively. For the

sake of convenience, the different possible dimers formed by different combinations of the monomeric units will be labelled with respect to the R groups as R_1R_2, i.e., dimer formed by combination of PA-2H and PA-BrCl will be labelled as (2H-BrCl).

Dimer	$\nu_{O\text{-}D}$	$\Delta\nu_{O\text{-}D}$	Field	$\nu_{O\text{-}D}$	$\Delta\nu_{O\text{-}D}$	Field
	On PA-2H due to partner			On partner due to PA-2H		
2H-2H	1855	-803	-111.49	1865	-793	-111.49
2H-HF	1981	-677	-97.07	1546	-1117	-114.63
2H-HCl	1979	-679	-96.11	1591	-1061	-115.58
2H-HBr	1972	-686	-95.21	1594	-1059	-115.70
2H-2F	1981	-677	-85.48	1387	-1283	-115.31
2H-2Cl	1967	-691	-84.68	1337	-1305	-116.11
2H-2Br	2005	-653	-84.57	1336	-1297	-114.34
2H-ClF	1995	-663	-85.45	1346	-1312	-116.10
2H-BrF	2012	-646	-85.01	1374	-1277	-116.37
2H-BrCl	2013	-645	-84.19	1366	-1277	-116.34
2H-HMe	1687	-971	-125.06	1903	-764	-112.69
2H-2Me	1575	-1083	-133.17	1986	-684	-108.68
2H-MeF	1900	-758	-109.65	1704	-966	-112.29
2H-MeCl	1918	-740	-106.21	1731	-931	-112.95
2H-MeBr	1937	-721	-103.98	1707	-955	-113.88
	On PA-HF due to partner			On partner due to PA-HF		
HF-HF	1815	-848	-98.58	1820	-843	-98.56
HF-2H	1546	-1117	-114.63	1981	-677	-97.07
HF-HCl	1774	-890	-97.62	1840	-812	-98.94
HF-HBr	1773	-890	-96.82	1865	-788	-98.93
HF-2F	1946	-718	-85.90	1654	-1016	-99.35
HF-2Cl	1911	-753	-85.61	1648	-993	-98.80
HF-2Br	1900	-763	-84.31	1633	-1001	-98.75
HF-ClF	1933	-730	-86.03	1654	-1003	-99.03
HF-BrF	1925	-738	-85.57	1653	-998	-99.14
HF-BrCl	1927	-736	-84.74	1610	-1034	-98.35
HF-HMe	1332	-1331	-126.95	1981	-686	-94.58
HF-2Me	1009	-1654	-139.13	2052	-618	-95.20
HF-MeF	1631	-1032	-110.99	1909	-761	-97.83
HF-MeCl	1623	-1040	-108.46	1909	-754	-98.30
HF-MeBr	1629	-1035	-107.06	1928	-734	-98.36
	On PA-HCl due to partner			On partner due to PA-HCl		
HCl-HCl	1838	-815	-98.06	1839	-814	-98.05
HCl-2H	1591	-1061	-115.58	1979	-679	-96.11
HCl-HF	1840	-812	-98.94	1774	-890	-97.62
HCl-HBr	1825	-828	-97.38	1836	-817	-98.23
HCl-2F	1987	-665	-86.43	1603	-1067	-98.84
HCl-2Cl	1945	-708	-86.63	1646	-996	-98.04
HCl-2Br	1910	-742	-84.77	1703	-930	-98.33
HCl-ClF	1954	-699	-86.61	1610	-1048	-98.67
HCl-BrF	1955	-697	-86.31	1633	-1018	-98.72
HCl-BrCl	1921	-731	-85.70	1667	-977	-98.51

HCl-HMe	1316	-1336	-128.16	2002	-665	-93.21
HCl-2Me	1000	-1652	-140.41	2055	-615	-93.53
HCl-MeF	1660	-993	-111.34	1918	-752	-96.32
HCl-MeCl	1671	-982	-108.70	1918	-744	-96.96
HCl-MeBr	1667	-985	-107.26	1930	-731	-96.87
	On PA-HBr due to partner			On partner due to PA-HBr		
HBr-HBr	1843	-810	-97.30	1840	-813	-97.29
HBr-2H	1594	-1059	-115.70	1972	-686	-95.21
HBr-HF	1865	-788	-98.93	1773	-890	-96.82
HBr-HCl	1836	-817	-98.23	1825	-828	-97.38
HBr-2F	1992	-661	-86.36	1604	-1067	-98.24
HBr-2Cl	1947	-706	-86.60	1608	-1034	-97.41
HBr-2Br	1933	-720	-84.86	1680	-953	-97.61
HBr-ClF	1968	-685	-86.68	1615	-1043	-98.06
HBr-BrF	1961	-692	-86.19	1638	-1012	-98.05
HBr-BrCl	1931	-722	-85.74	1672	-972	-97.81
HBr-HMe	1283	-1370	-128.50	2001	-666	-92.17
HBr-2Me	967	-1686	-140.63	901	-1769	-92.57
HBr-MeF	1737	-916	-111.29	1903	-767	-95.41
HBr-MeCl	1681	-972	-108.73	1914	-748	-96.00
HBr-MeBr	1701	-952	-107.37	1917	-745	-96.15
	On PA-2F due to partner			On partner due to PA-2F		
2F-2F	1881	-789	-86.03	1880	-790	-86.04
2F-2H	1387	-1283	-115.31	1981	-677	-85.48
2F-HF	1654	-1016	-99.35	1946	-718	-85.90
2F-HCl	1603	-1067	-98.84	1987	-665	-86.43
2F-HBr	1604	-1067	-98.24	1992	-661	-86.36
2F-2Cl	1719	-952	-86.27	1922	-720	-85.90
2F-2Br	1722	-948	-84.84	1903	-730	-85.78
2F-ClF	1827	-843	-86.54	1909	-749	-86.07
2F-BrF	1815	-855	-86.03	1912	-739	-86.21
2F-BrCl	1722	-948	-85.44	1906	-738	-85.34
2F-HMe	976	-1694	-128.69	2171	-496	-82.63
2F-2Me	600	-2070	-140.80	2093	-578	-85.70
2F-MeF	1452	-1218	-112.25	1990	-680	-85.62
2F-MeCl	1429	-1241	-110.25	1998	-665	-86.19
2F-MeBr	1434	-1236	-108.89	2004	-658	-86.17
	On PA-2Cl due to partner			On partner due to PA-2Cl		
2Cl-2Cl	1824	-818	-86.67	1831	-811	-86.67
2Cl-2H	1337	-1305	-116.11	1967	-691	-84.68
2Cl-HF	1648	-993	-98.80	1911	-753	-85.61
2Cl-HCl	1646	-996	-98.04	1945	-708	-86.63
2Cl-HBr	1608	-1034	-97.41	1947	-706	-86.60
2Cl-2F	1922	-720	-85.90	1719	-952	-86.27
2Cl-2Br	1789	-853	-84.46	1850	-784	-85.66
2Cl-ClF	1873	-768	-85.77	1834	-824	-85.86
2Cl-BrF	1859	-782	-85.49	1804	-847	-86.09
2Cl-BrCl	1801	-840	-85.39	1843	-801	-85.85

2Cl-HMe	1047	-1594	-128.20	2044	-623	-85.20
2Cl-2Me	613	-2029	-141.38	2038	-632	-84.33
2Cl-MeF	1460	-1182	-111.71	1963	-707	-85.01
2Cl-MeCl	1450	-1191	-109.60	1958	-705	-85.59
2Cl-MeBr	1397	-1244	-107.90	1988	-674	-85.78
	On PA-2Br due to partner			On partner due to PA-2Br		
2Br-2Br	1785	-848	-85.43	1783	-851	-85.43
2Br-2H	1336	-1297	-114.34	2005	-653	-84.57
2Br-HF	1633	-1001	-98.75	1900	-763	-84.31
2Br-HCl	1703	-930	-98.33	1910	-742	-84.77
2Br-HBr	1680	-953	-97.61	1933	-720	-84.86
2Br-2F	1903	-730	-85.78	1722	-948	-84.84
2Br-2Cl	1850	-784	-85.66	1789	-853	-84.46
2Br-ClF	1823	-811	-86.60	1829	-829	-85.34
2Br-BrF	1873	-761	-86.03	1784	-867	-85.62
2Br-BrCl	1815	-819	-84.76	1797	-847	-84.09
2Br-HMe	985	-1648	-128.71	2151	-515	-80.89
2Br-2Me	262	-2372	-140.69	2043	-627	-83.35
2Br-MeF	1426	-1207	-111.50	1964	-706	-84.06
2Br-MeCl	1413	-1220	-109.19	1967	-696	-84.40
2Br-MeBr	1461	-1172	-107.83	1968	-694	-84.33
	On PA-ClF due to partner			On partner due to PA-ClF		
ClF-ClF	1859	-798	-86.22	1861	-797	-85.81
ClF-2H	1346	-1312	-116.10	1995	-663	-85.45
ClF-HF	1654	-1003	-99.03	1933	-730	-86.03
ClF-HCl	1610	-1048	-98.67	1954	-699	-86.61
ClF-HBr	1615	-1043	-98.06	1968	-685	-86.68
ClF-2F	1909	-749	-86.07	1827	-843	-86.54
ClF-2Cl	1834	-824	-85.86	1873	-768	-85.77
ClF-2Br	1829	-829	-85.34	1823	-811	-86.60
ClF-BrF	1816	-842	-85.44	1857	-793	-86.59
ClF-BrCl	1756	-902	-86.27	1847	-797	-86.25
ClF-HMe	1007	-1651	-127.96	907	-1760	-82.03
ClF-2Me	448	-2210	-140.22	2087	-583	-84.74
ClF-MeF	1476	-1181	-111.91	1970	-700	-85.84
ClF-MeCl	1439	-1219	-109.63	1966	-696	-86.31
ClF-MeBr	1438	-1220	-108.34	2005	-657	-86.35
	On PA-BrF due to partner			On partner due to PA-BrF		
BrF-BrF	1847	-804	-85.99	1854	-797	-86.07
BrF-2H	1374	-1277	-116.37	2012	-646	-85.01
BrF-HF	1653	-998	-99.14	1925	-738	-85.57
BrF-HCl	1633	-1018	-98.72	1955	-697	-86.31
BrF-HBr	1638	-1012	-98.05	1961	-692	-86.19
BrF-2F	1912	-739	-86.21	1815	-855	-86.03
BrF-2Cl	1804	-847	-86.09	1859	-782	-85.49
BrF-2Br	1784	-867	-85.62	1873	-761	-86.03
BrF-ClF	1857	-793	-86.59	1816	-842	-85.44
BrF-BrCl	1828	-823	-86.26	1836	-808	-86.22

BrF-HMe	1045	-1606	-128.25	2158	-509	-81.24
BrF-2Me	404	-2247	-140.43	2111	-559	-83.69
BrF-MeF	1489	-1162	-112.05	1977	-693	-85.16
BrF-MeCl	1459	-1192	-109.68	1988	-674	-85.72
BrF-MeBr	1474	-1177	-108.30	2014	-647	-85.65
	On PA-BrCl due to partner			On partner due to PA-BrCl		
BrCl-BrCl	1849	-795	-85.57	1855	-789	-85.58
BrCl-2H	1366	-1277	-116.34	2013	-645	-84.19
BrCl-HF	1610	-1034	-98.35	1927	-736	-84.74
BrCl-HCl	1667	-977	-98.51	1921	-731	-85.70
BrCl-HBr	1672	-972	-97.81	1931	-722	-85.74
BrCl-2F	1906	-738	-85.34	1722	-948	-85.44
BrCl-2Cl	1843	-801	-85.85	1801	-840	-85.39
BrCl-2Br	1797	-847	-84.09	1815	-819	-84.76
BrCl-ClF	1847	-797	-86.25	1756	-902	-86.27
BrCl-BrF	1836	-808	-86.22	1828	-823	-86.26
BrCl-HMe	894	-1750	-130.00	2154	-512	-80.69
BrCl-2Me	362	-2282	-140.61	2090	-581	-83.70
BrCl-MeF	1482	-1162	-111.88	1954	-716	-84.76
BrCl-MeCl	1438	-1206	-109.42	1969	-694	-85.17
BrCl-MeBr	1481	-1163	-108.06	1982	-680	-85.15
	On PA-HMe due to partner			On partner due to PA-HMe		
HMe-HMe	1861	-806	-122.97	1863	-803	-122.96
HMe-2H	1903	-764	-112.69	1687	-971	-125.06
HMe-HF	1981	-686	-94.58	1332	-1331	-126.95
HMe-HCl	2002	-665	-93.21	1316	-1336	-128.16
HMe-HBr	2001	-666	-92.17	1283	-1370	-128.50
HMe-2F	2171	-496	-82.63	976	-1694	-128.69
HMe-2Cl	2044	-623	-85.20	1047	-1594	-128.20
HMe-2Br	2151	-515	-80.89	985	-1648	-128.71
HMe-ClF	2167	-500	-82.03	1007	-1651	-127.96
HMe-BrF	2158	-509	-81.24	1045	-1606	-128.25
HMe-BrCl	2154	-512	-80.69	894	-1750	-130.00
HMe-2Me	1719	-948	-134.20	1918	-752	-121.87
HMe-MeF	2028	-638	-105.70	1534	-1136	-125.25
HMe-MeCl	2009	-658	-102.61	1488	-1174	-125.81
HMe-MeBr	2014	-653	-101.54	1522	-1139	-125.76
	On PA-2Me due to partner			On partner due to PA-2Me		
2Me-2Me	1807	-863	-129.01	1808	-863	-129.00
2Me-2H	1986	-684	-108.68	1575	-1083	-133.17
2Me-HF	2052	-618	-95.20	1009	-1654	-139.13
2Me-HCl	2055	-615	-93.53	1000	-1652	-140.41
2Me-HBr	2059	-611	-92.57	967	-1686	-140.63
2Me-2F	2093	-578	-85.70	600	-2070	-140.80
2Me-2Cl	2038	-632	-84.33	613	-2029	-141.38
2Me-2Br	2043	-627	-83.35	262	-2372	-140.69
2Me-ClF	2087	-583	-84.74	448	-2210	-140.22
2Me-BrF	2111	-559	-83.69	404	-2247	-140.43

2Me-BrCl	2090	-581	-83.70	362	-2282	-140.61
2Me-HMe	1918	-752	-121.87	1719	-948	-134.20
2Me-MeF	1945	-725	-105.85	1286	-1384	-137.17
2Me-MeCl	1935	-735	-102.93	1274	-1388	-138.35
2Me-MeBr	1921	-750	-101.35	1244	-1418	-138.65
	On PA-MeF due to partner			On partner due to PA-MeF		
MeF-MeF	1741	-929	-109.91	1741	-929	-109.91
MeF-2H	1704	-966	-112.29	1900	-758	-109.65
MeF-HF	1909	-761	-97.83	1631	-1032	-110.99
MeF-HCl	1918	-752	-96.32	1660	-993	-111.34
MeF-HBr	1903	-767	-95.41	1737	-916	-111.29
MeF-2F	1990	-680	-85.62	1452	-1218	-112.25
MeF-2Cl	1963	-707	-85.01	1460	-1182	-111.71
MeF-2Br	1964	-706	-84.06	1426	-1207	-111.50
MeF-ClF	1970	-700	-85.84	1476	-1181	-111.91
MeF-BrF	1977	-693	-85.16	1489	-1162	-112.05
MeF-BrCl	1954	-716	-84.76	1482	-1162	-111.88
MeF-HMe	1534	-1136	-125.25	2028	-638	-105.70
MeF-2Me	1286	-1384	-137.17	1945	-725	-105.85
MeF-MeCl	1730	-940	-107.26	1749	-913	-110.55
MeF-MeBr	1753	-917	-105.76	1739	-923	-110.81
	On PA-MeCl due to partner			On partner due to PA-MeCl		
MeCl-MeCl	1757	-906	-107.63	1757	-906	-107.62
MeCl-2H	1731	-931	-112.95	1918	-740	-106.21
MeCl-HF	1909	-754	-98.30	1623	-1040	-108.46
MeCl-HCl	1918	-744	-96.96	1671	-982	-108.70
MeCl-HBr	1914	-748	-96.00	1681	-972	-108.73
MeCl-2F	1998	-665	-86.19	1429	-1241	-110.25
MeCl-2Cl	1958	-705	-85.59	1450	-1191	-109.60
MeCl-2Br	1967	-696	-84.40	1413	-1220	-109.19
MeCl-ClF	1966	-696	-86.31	1439	-1219	-109.63
MeCl-BrF	1988	-674	-85.72	1459	-1192	-109.68
MeCl-BrCl	1969	-694	-85.17	1438	-1206	-109.42
MeCl-HMe	1488	-1174	-125.81	2009	-658	-102.61
MeCl-2Me	1274	-1388	-138.35	1935	-735	-102.93
MeCl-MeF	1749	-913	-110.55	1730	-940	-107.26
MeCl-MeBr	1733	-930	-106.53	1748	-914	-108.18
	On PA-MeBr due to partner			On partner due to PA-MeBr		
MeBr-MeBr	1773	-889	-106.28	1756	-906	-106.30
MeBr-2H	1707	-955	-113.88	1937	-721	-103.98
MeBr-HF	1928	-734	-98.36	1629	-1035	-107.06
MeBr-HCl	1930	-731	-96.87	1667	-985	-107.26
MeBr-HBr	1917	-745	-96.15	1701	-952	-107.37
MeBr-2F	2004	-658	-86.17	1434	-1236	-108.89
MeBr-2Cl	1988	-674	-85.78	1397	-1244	-107.90
MeBr-2Br	1968	-694	-84.33	1461	-1172	-107.83

MeBr-ClF	2005	-657	-86.35	1438	-1220	-108.34
MeBr-BrF	2014	-647	-85.65	1474	-1177	-108.30
MeBr-BrCl	1982	-680	-85.15	1481	-1163	-108.06
MeBr-HMe	1522	-1139	-125.76	2014	-653	-101.54
MeBr-2Me	1244	-1418	-138.65	1921	-750	-101.35
MeBr-MeF	1739	-923	-110.81	1753	-917	-105.76
MeBr-MeCl	1748	-914	-108.18	1733	-930	-106.53

Table S7. The harmonic vibrational frequencies (in cm^{-1}) of the donor O-D stretch along with its vibrational shift (in cm^{-1}) with respect to O-D stretch of the corresponding phosphinic acid monomer and the electric field (in MV cm^{-1}) along the bond calculated at B3LYP-D3/TZVP level of theory for the two cases namely, the effect on acid due to partner and the effect on partner due to acid respectively. For the sake of convenience, the different possible dimers formed by different combinations of the monomeric units will be labelled with respect to the R groups as R_1R_2, i.e., dimer formed by combination of PA-HH and PA-ClF will be labelled as (2H-ClF).

Dimer	$\nu_{O\text{-}D}$	$\Delta\nu_{O\text{-}D}$	Field	$\nu_{O\text{-}D}$	$\Delta\nu_{O\text{-}D}$	Field
	On PA-2H due to partner			On partner due to PA-2H		
2H-2H	2194	-581	-120.50	2194	-581	-120.49
2H-HF	2317	-458	-104.13	1987	-783	-126.31
2H-HCl	2290	-485	-103.54	1999	-764	-126.75
2H-HBr	2303	-472	-101.88	2015	-748	-126.38
2H-2F	2385	-390	-92.58	1843	-938	-128.73
2H-2Cl	2375	-400	-91.26	1819	-936	-128.03
2H-2Br	2383	-392	-89.26	1835	-910	-128.78
2H-ClF	2376	-399	-92.07	1846	-923	-129.19
2H-BrF	2373	-402	-92.07	1863	-905	-128.95
2H-BrCl	2367	-408	-90.57	1841	-909	-128.89
2H-HMe	2112	-663	-132.36	2201	-577	-121.26
2H-2Me	2021	-754	-140.77	2256	-525	-118.25
	On PA-ClF due to partner			On partner due to PA-ClF		
ClF-ClF	1846	-923	-129.19	2376	-399	-92.07
ClF-2H	2068	-701	-109.76	2244	-526	-94.42
ClF-HF	2048	-721	-108.51	2271	-492	-94.36
ClF-HCl	2031	-738	-108.15	2285	-478	-94.20
ClF-HBr	2206	-563	-95.51	2169	-612	-95.52
ClF-2F	2162	-607	-94.78	2170	-585	-95.01
ClF-2Cl	2147	-622	-93.67	2192	-553	-94.50
ClF-2Br	2191	-578	-95.32	2189	-580	-95.32
ClF-BrF	2181	-588	-95.40	2208	-560	-95.10
ClF-BrCl	2154	-615	-94.48	2162	-588	-94.80
ClF-HMe	1695	-1074	-138.01	2452	-326	-89.46
ClF-2Me	1493	-1276	-150.69	2443	-338	-91.16

Table S8. The harmonic vibrational frequencies (in cm^{-1}) of the donor O-D stretch along with its vibrational shift (in cm^{-1}) with respect to O-D stretch of the corresponding phosphinic acid monomer and the electric field (in MV cm^{-1}) along the bond calculated at B2GP-PLYP-D3/def2-TZVP/CP level of theory for the two cases namely, the effect on acid due to partner and the effect on partner due to acid respectively. For the sake of convenience, the different possible dimers formed by different combinations of the monomeric units will be labelled with respect to the R groups as R_1R_2, i.e., dimer formed by combination of PA-HH and PA-ClF will be labelled as (2H-ClF).

Dimer	$\nu_{O\text{-}D}$	$\Delta\nu_{O\text{-}D}$	Field	$\nu_{O\text{-}D}$	$\Delta\nu_{O\text{-}D}$	Field
	On PA-2H due to partner			On partner due to PA-2H		
2H-2H	2286	-537	-133.67	2286	-537	-133.66
2H-HF	2412	-411	-113.48	2118	-699	-139.40
2H-HCl	2406	-417	-113.17	2127	-682	-139.80
2H-HBr	2435	-388	-111.47	2086	-721	-140.63
2H-2F	2481	-342	-100.09	2002	-827	-142.83
2H-2Cl	2463	-360	-101.17	1963	-835	-141.99
2H-2Br	2417	-406	-102.40	1999	-792	-141.88
2H-ClF	2458	-365	-102.04	1984	-834	-143.87
2H-BrF	2486	-337	-100.38	1987	-824	-144.10
2H-BrCl	2459	-364	-102.74	1973	-820	-142.78
2H-HMe	2229	-594	-143.79	2302	-520	-132.96
2H-2Me	2158	-665	-152.50	2321	-501	-130.41
	On PA-ClF due to partner			On partner due to PA-ClF		
ClF-ClF	1983	-835	-143.86	2458	-365	-102.05
ClF-2H	2185	-633	-121.17	2337	-480	-104.48
ClF-HF	2170	-648	-121.67	2358	-451	-104.66
ClF-HCl	2141	-677	-121.10	2383	-424	-104.04
ClF-HBr	2337	-481	-104.18	2271	-558	-106.99
ClF-2F	2268	-550	-108.39	2282	-516	-105.55
ClF-2Cl	2206	-612	-109.48	2293	-498	-105.18
ClF-2Br	2265	-553	-106.21	2318	-500	-106.21
ClF-BrF	2264	-554	-104.95	2296	-515	-107.25
ClF-BrCl	2256	-562	-107.42	2267	-526	-105.90
ClF-HMe	1895	-923	-152.70	2476	-346	-100.26
ClF-2Me	1674	-1144	-166.38	2506	-316	-100.98

Table S9. Fitting parameters for linear least-square fits for the plots shown in Figures 3, 4, S3 and S4 for the O–H and O–D shifts of R due to R′.

	MP2 (Harmonic)			MP2 (Harmonic)			B3LYP (Harmonic)			B3LYP (Anharmonic)		
	O–H			O–D			O–D			O–D		
	Slope	Residual	R^2	Slope	Residual	R^2	Slope	Residual	R^2	Slope	Residual	R^2
2H	8.9	20.9	0.995	6.2	15.5	0.994	7.0	32.9	0.976	7.5	87.3	0.853
HF	11.2	89.3	0.971	7.7	49.1	0.978	9.2	54.7	0.966	15.3	115.6	0.962
HCl	11.8	87.0	0.976	8.2	48.9	0.982	9.6	54.7	0.969	15.7	128.9	0.948
HBr	12.0	88.7	0.975	8.3	50.2	0.980	9.7	57.5	0.969	16.1	151.6	0.927
2F	14.4	145.1	0.955	9.8	84.3	0.965	12.2	100.8	0.951	19.0	181.0	0.921
2Cl	14.5	152.3	0.957	9.9	93.6	0.964	13.1	117.2	0.947	20.0	142.8	0.960
2Br	15.1	150.5	0.961	10.3	87.8	0.971	12.8	113.2	0.953	24.0	323.9	0.912
ClF	14.2	169.0	0.947	9.7	103.2	0.957	12.4	113.9	0.946	21.7	249.8	0.926
BrF	13.7	126.9	0.968	9.4	81.4	0.973	12.1	105.0	0.955	21.9	299.5	0.907
BrCl	14.5	139.5	0.957	10.0	86.3	0.964	12.3	112.5	0.944	22.9	282.8	0.916
HMe	8.1	64.6	0.974	6.0	44.3	0.975	7.0	48.5	0.963	7.6	66.4	0.905
2Me	7.1	17.1	0.994	5.3	22.3	0.987	6.3	20.5	0.987	5.5	65.5	0.817
MeF	9.8	53.1	0.980	6.9	40.6	0.978	8.0	40.6	0.972	12.0	87.5	0.952
MeCl	10.5	51.9	0.983	7.4	40.4	0.981	8.5	38.7	0.975	12.3	81.5	0.946
MeBr	10.8	47.5	0.987	7.7	37.6	0.985	8.8	33.6	0.980	12.8	100.1	0.949
Average	**11.8 (σ=2.6)**			**8.2 (σ=1.6)**			**10.0 (σ=2.4)**			**15.4 (σ=5.8)**		

Table S10. Fitting parameters for linear least-square fits for the plots shown in Figures 3, 4, S3 and S4 for the O–H and O–D shifts of R′ due to R.

	MP2 (Harmonic)			MP2 (Harmonic)			B3LYP (Harmonic)			B3LYP (Anharmonic)		
	O–H			O–D			O–D			O–D		
	Slope	Residual	R^2	Slope	Residual	R^2	Slope	Residual	R^2	Slope	Residual	R^2
2H	44.5	84.0	0.925	31.8	60.9	0.923	57.9	107.1	0.789	86.1	210.3	0.738
HF	45.4	79.7	0.885	32.8	55.4	0.883	68.1	83.0	0.754	73.3	166.4	0.472
HCl	39.8	83.9	0.914	28.7	58.1	0.913	62.3	65.7	0.875	71.5	106.2	0.696
HBr	38.7	82.8	0.917	27.9	57.3	0.917	60.1	98.2	0.888	68.8	761.4	0.728
2F	48.0	100.3	0.794	34.9	69.5	0.807	57.4	167.4	0.288	52.9	105.5	0.391
2Cl	46.3	105.5	0.83	33.9	72.9	0.84	101.	164.3	0.41	68.2	166.4	0.23

			3			9	2		0			3
2Br	48.4	107.9	0.867	35.2	74.7	0.878	73.6	127.4	0.533	75.2	157.8	0.525
ClF	43.0	88.8	0.862	31.1	61.6	0.868	62.0	192.9	0.498	59.6	421.2	0.545
BrF	43.4	96.4	0.817	31.7	67.6	0.827	60.8	101.8	0.581	56.6	122.0	0.523
BrCl	44.1	113.5	0.867	31.9	79.2	0.871	63.1	122.8	0.612	65.2	170.5	0.553
HMe	55.2	130.1	0.931	37.9	84.6	0.940	76.4	130.6	0.860	133.4	181.3	0.891
2Me	55.7	177.2	0.896	37.4	104.1	0.909	68.2	174.0	0.762	130.4	516.0	0.676
MeF	44.8	98.6	0.907	31.3	69.8	0.904	61.1	96.5	0.834	79.6	170.6	0.731
MeCl	43.6	80.9	0.928	30.5	59.2	0.924	57.5	66.0	0.890	76.1	141.7	0.793
MeBr	42.5	75.8	0.935	29.7	54.2	0.930	56.6	66.2	0.905	75.2	130.3	0.809
Average	**45.6 (σ=4.8)**			**32.4 (σ=2.9)**			**65.7 (σ=11.5)**			**78.1 (σ=23.5)**		

Table S11. Fitting parameters for linear least-square fits for the plots shown in Figure S5 for the harmonic O–D shifts of R due to R′ as well as R′ due to R. The values shown in parenthesis were calculated at MP2/aug-cc-pVDZ level.

	B3LYP/TZVP						B2GP-PLYP-D3/def2-TZVP/CP					
	R due to R′			R′ due to R			R due to R′			R′ due to R		
	Slope	Residual	R^2	Slope	Residual	R^2	Slope	Residual	R^2	Slope	Residual	R^2
2H	6.8	24.9	0.987	39.5	64.5	0.937	5.8 (6.2)	44.9	0.972	27.6 (31.8)	51.0	0.957
ClF	11.4	53.0	0.972	50.1	43.7	0.917	9.1 (9.7)	63.4	0.965	33.0 (31.1)	35.1	0.917

Table S12. Comparison of O–H vibrational frequency shifts for various phosphinic acid dimer in presence of an external electric field equivalent to the value in the hydrogen-bonded dimer against the corresponding red-shift in the hydrogen-bonded dimer.

2H		**HF**		**HCl**		**HBr**	
-556.6	-100.4	-587.4	-75.8	-588.5	-77.8	-587.8	-78.1
-432.8	-80.0	-756.3	-100.3	-746.5	-100.3	-736.7	-99.5
-450.0	-81.4	-614.1	-78.6	-558.9	-75.7	-547.6	-76.4
-455.8	-81.0	-620.0	-78.1	-595.4	-77.4	-578.4	-78.1
-332.1	-64.5	-484.1	-59.2	-445.6	-58.9	-428.7	-59.5
-376.9	-70.5	-538.6	-65.8	-494.5	-65.8	-475.1	-65.9
-380.5	-70.5	-557.2	-66.3	-525.6	-65.8	-510.5	-66.4
-338.4	-65.9	-508.4	-62.1	-472.9	-61.8	-456.8	-62.8
-343.3	-65.9	-513.9	-62.6	-481.3	-62.6	-463.2	-63.3
-375.4	-69.1	-552.2	-66.3	-502.6	-65.8	-502.1	-66.4
-651.4	-114.7	-885.2	-116.8	-873.4	-116.3	-872.3	-114.9
-720.4	-125.5	-1038.4	-133.1	-1038.5	-131.6	-1037.8	-129.4
-507.8	-93.6	-674.6	-89.5	-645.9	-89.5	-628.2	-88.4
-506.7	-92.3	-702.1	-90.1	-672.0	-89.1	-661.0	-89.4
-502.3	-89.5	-705.1	-89.0	-679.2	-88.9	-667.7	-88.4
HMe		2F		BrF		MeF	
-555.6	-94.7	-547.0	-52.5	-537.8	-57.2	-616.2	-69.5
-557.8	-86.2	-881.3	-97.4	-856.4	-92.3	-666.1	-77.4
-368.2	-64.2	-671.8	-70.6	-642.7	-69.6	-537.8	-58.6
-373.6	-64.6	-711.7	-74.1	-673.8	-71.7	-558.1	-59.9
-375.2	-63.8	-722.0	-74.1	-678.6	-71.7	-562.2	-59.5
-271.6	-51.0	-621.8	-59.8	-525.1	-54.5	-452.6	-44.2
-286.8	-55.9	-644.0	-60.4	-570.7	-60.1	-497.5	-50.1
-299.3	-55.9	-580.5	-56.3	-584.5	-61.3	-508.9	-50.1
-280.9	-64.2	-588.0	-56.8	-562.4	-58.6	-473.5	-47.6
-273.3	-53.5	-633.5	-59.5	-573.2	-60.8	-477.4	-47.6
-292.4	-55.9	-1074.0	-118.1	-981.3	-105.6	-501.4	-50.1
-633.1	-105.2	-1299.4	-141.2	-1222.6	-119.3	-791.3	-91.3
-405.2	-74.4	-787.5	-85.3	-756.1	-82.0	-926.1	-103.9
-409.3	-73.9	-829.5	-86.6	-772.1	-82.0	-642.6	-69.7
-412.5	-73.1	-831.7	-85.3	-785.2	-81.2	-644.9	-69.2