

[H₂O-PH₃]⁺

HB:

H	-0.7079069842	-1.1447359058	0.7406138401
P	-0.8543552873	-0.0000841313	-0.0368048977
H	-2.1371745582	0.0018931946	-0.6023189121
H	-0.7051946002	1.1437350452	0.7414209247
H	2.0800964360	-0.7785038808	-0.2009032369
O	1.5259771517	-0.0003342079	0.0092010813
H	2.0756036197	0.7819868547	-0.1971919063

HYB:

H	-0.2422800144	-0.0015965380	-0.0230856854
P	1.1867808954	-0.0000179593	-0.0660266091
H	1.8140130257	-1.1463159638	0.4226825871
H	1.8103702718	1.1531998906	0.4108523011
H	-2.5793978668	0.0068536110	0.7999990619
O	-2.0001372140	0.0031905165	0.0155170203
H	-2.5988001360	-0.0054641811	-0.7543525794

PT

H	2.0270073538	-1.0527968511	-0.1546060572
P	1.1143694020	0.0000177021	0.0063066324
H	-0.8352683841	0.0006425560	-0.0047348864
H	1.9632636693	1.1006938740	0.1918456004
H	-2.3216279532	-0.4258289981	0.7328865037
O	-1.9093149097	0.0867242315	-0.0016714609
H	-2.3065449136	-0.1850373999	-0.8622688791

[H₂O-H₂S]⁺

HB

H	2.1432848182	-0.7449363925	-0.0015844111
O	1.5189025831	0.0067517758	-0.0318722935
H	2.0209182594	0.7904852422	0.2657953612
H	-0.7469132316	-0.3370644122	-1.2264593775
S	-0.9218554578	0.0858473753	0.0391198731
H	-0.8195128511	-1.1351758267	0.5956551299

HYB

H	-2.3958682524	-0.0964043848	0.7826458517
O	-1.8258743060	0.0371916624	0.0004707265
H	-2.3946188436	-0.0789361372	-0.7853884977
H	-0.2797595333	-0.0611275312	-0.0007554463
S	1.1492473736	-0.0825207368	-0.0006337560
H	1.2892830995	1.2592665424	0.0098723769

PT

H	-2.2268701884	-0.1720186524	0.8384133129
O	-1.8095889994	0.0969736849	-0.0131974356
H	-2.2244311912	-0.4075926886	-0.7514976282
H	-0.7155509413	0.0047045932	0.0018823522
S	1.1397820053	-0.0887796863	0.0121127528
H	1.4038100007	1.2253796987	-0.1210648881

[H₂O-HCl]⁺

HB

H	-1.7618595130	-0.3844336838	0.7885104437
O	-1.4237243621	0.1043289581	0.0007361508
H	-1.7627651020	-0.3736018302	-0.7932667654
H	0.7645749593	1.2201457387	0.0052802423
Cl	0.8322978337	-0.0762474571	-0.0006781912

PT

H	2.2708173766	-0.8110153970	0.3174453844
O	1.8807114604	0.0000280155	-0.0917697541
H	2.2703748513	0.8112348118	0.3175485584
H	0.8656302090	-0.0002024723	-0.0293891087
Cl	-1.2104305510	0.0003852895	0.0152017347

[(H₂O)₂-PH₃]⁺

PT

H	-0.1126244921	-0.6175230106	0.0269628157
P	-2.0704744664	0.2210923812	-0.0071074271
H	-3.0568792636	0.0771433704	-0.9978683198
H	-2.7634393326	1.0570868973	0.8856310059
H	0.8906079779	-1.7398615140	0.6878859563
O	0.8086289774	-1.0577924061	-0.0132542464
H	1.5949156490	-0.3650041660	0.0223230613
H	3.0935686846	1.1130258314	0.7077105714
O	2.7035888224	0.6159591255	-0.0349915892
H	3.3395270041	0.6419740670	-0.7743442807

HB

H	0.9200566724	-1.0335302618	0.9538273315
P	1.5495619090	-0.2917265045	-0.0413332574
H	2.2513754406	0.7508659345	0.5570079487
H	2.5275376262	-1.1450874404	-0.5918897279
H	-2.9872217293	-0.7207311570	-0.7757415048
O	-2.4726939087	-0.4219998398	-0.0039797563
H	-3.1073309201	-0.3581677695	0.7330357078
H	-1.0983382562	0.5263908824	-0.0372549318
O	-0.2092871748	0.9915767647	0.0434440523
H	-0.2388283017	1.7935200619	-0.5176821721

HB

H	0.0131794886	0.0897623712	-1.1569023314
P	-0.0789100527	-0.6559991223	0.0097567037
H	0.0172142336	0.1175206040	1.1579015362
H	0.8739607640	-1.6764250887	0.0219534089
H	-2.9365094365	0.5946440480	-0.7662564167
O	-2.3304339398	0.5293520197	-0.0043129500
H	-2.8802137110	0.7294936961	0.7768381733
H	2.5639065007	1.4790898002	-0.1170752208
O	2.3668437678	0.5308731034	-0.0046571089
H	3.2384887148	0.1056359965	0.0944217028

HYD

H	1.2153024028	0.1570471715	0.0380455060
P	0.0000669161	0.8858674185	0.0799728538
H	-1.2196368833	0.1677699335	0.0081697216

H	0.0142720654	2.0370670690	-0.7076170101
H	3.2161589096	-1.2502800640	-0.7093482958
O	2.8427338495	-0.7043052300	0.0062761438
H	3.5062644315	-0.7256785724	0.7198496535
H	-3.4869588071	-0.7822430141	0.6937034875
O	-2.8409788858	-0.7137146500	-0.0327797808
H	-3.2350313492	-1.2055322206	-0.7760174729

[(H₂O)₂-H₂S]⁺

PT

H	-3.0004421238	1.0862198619	0.7189615259
O	-2.6238591698	0.5898174098	-0.0312514075
H	-3.2756690098	0.6137927827	-0.7567818604
H	-1.5112472020	-0.3921013134	0.0079355318
O	-0.7183739075	-1.0756011899	-0.0408216525
H	-0.8012370029	-1.7659997415	0.6521967671
H	0.2023050494	-0.6206574535	0.0120767187
S	2.0285975654	0.3295438985	0.0582995141
H	2.7022739832	-0.3745323756	-0.8698039425

HYD

H	2.2017029831	-1.8765387393	0.0164288981
O	2.2650423589	-0.9035053555	0.0122821469
H	3.2173385635	-0.6921353916	0.0170215833
H	-2.7936445894	-1.1566154309	-0.7845224580
O	-2.2714995829	-0.8846200576	-0.0067132767
H	-2.7992053145	-1.1400872346	0.7729562507
H	-1.0418710303	0.2683078975	-0.0087856713
S	0.0148961774	1.1726419760	-0.0030665532
H	1.0213100811	0.2119430993	0.0090930950

HB

H	0.9623761086	-1.1900414189	-0.1178658931
O	0.0346803197	-1.4606823833	0.0703694997
H	-0.1746874772	-2.2366125856	-0.4868806240
H	2.5239526014	0.8546414565	-0.7438841945
O	1.9801124417	0.5260923145	-0.0023246211
H	2.5528533533	0.6183924613	0.7834007456
H	-0.0158636996	0.9941839754	0.0846326872
S	-1.2735174794	0.5182753672	-0.0833614263
H	-1.4678516316	0.2126126156	1.2111916683

[(H₂O)₂-HCl]⁺

PT

H	-3.0838292423	-0.9362414104	0.8041199194
O	-2.6260015001	-0.6204535595	0.0015882444
H	-3.2494581711	-0.6918042644	-0.7471773603
H	0.0995623021	0.6206327307	-0.0326876369
Cl	2.1201080752	-0.2854174952	0.0329715427
H	-0.8605173946	1.7934655273	0.5395850221
O	-0.7964685555	1.0504125069	-0.0990777065
H	-1.6092666866	0.3467671239	-0.0065538502

PT

H	1.6025523658	-0.3642600250	-0.0983124107
O	2.8588193305	0.6347340817	0.0937513946
H	3.3700816012	1.0896093000	-0.6167192391
H	-0.0698332624	-0.5938523782	-0.0666173223
Cl	-1.9166411105	0.3141983721	0.0457774988
H	-2.6098796061	-0.1719223280	-0.9232281030
O	0.8328664316	-1.0442604834	-0.1011350780
H	0.9242505259	-1.6675090212	0.6563030330

HB

H	1.0321481667	0.5038576193	0.0075282581
O	0.1639094999	1.0187948200	-0.0613616757
H	0.1478093711	1.6685990261	0.6732402368
H	2.8907872125	-0.7651100650	0.7286344490
Cl	-1.5095614789	-0.3568039392	0.0826518710
H	-1.7725083670	0.1535609598	-1.0791609121
O	2.4038315652	-0.3954685728	-0.0300629660
H	3.0604924178	-0.2704283711	-0.7394720112

HB

H	-2.1548581448	-1.0780223075	0.6863084366
O	-1.5482181144	-0.9809230532	-0.0893725535
H	-0.6312957591	-1.1828904808	0.2328118619
H	-0.4903052976	1.1438576457	-0.0834934836
Cl	1.6022872030	-0.0379914504	-0.0554997403
H	2.2687285827	0.2325711345	1.0113767886
O	-1.4599997977	1.0334784754	0.0993126057
H	-1.9334826831	1.2122468249	-0.7496811527

[H₂O-(PH₃)₂]⁺

HB

H	2.7983362274	-0.7244549939	0.0550437950
P	1.5399128249	-0.0982250536	-0.0026792784
H	1.5968764722	0.6163444855	-1.2019434196
H	1.6270357697	0.9055555250	0.9674968475
H	-1.3444144200	-0.6968935794	1.3052041973
P	-1.0299371823	-1.0159425759	-0.0179122400
H	-0.9602233214	-2.4162865216	0.0054389872
H	-2.2210323388	-0.7526313621	-0.7163185415
H	-1.0980534994	2.3794489587	-0.7944750042
O	-0.8674751752	1.8604703185	-0.0014858414
H	-1.0978048263	2.4465047530	0.7435844927

PT

H	0.6801116512	-0.2285445279	-1.1438820316
P	0.8815013798	-0.9728015479	0.0082693563
H	0.6794272041	-0.2106965441	1.1484457158
H	2.1625848347	-1.5119518590	0.0142529382
H	-0.0218719464	-2.0319530805	0.0167301042
P	-2.4666682998	0.3383243355	0.0033432200
H	-3.3928169917	0.5444800829	-1.0406016466
H	-3.3149076114	0.7831704244	1.0390350436
H	2.4292970428	2.0549037912	0.0514832026
O	2.6424565857	1.1059416410	-0.0146985252
H	3.6136928462	1.0789047063	-0.0947447968

PT

H	-3.3635905512	-1.1598200858	0.9395848168
P	-2.7274635412	-0.3237192431	0.0047308117
H	-0.8514407393	0.7404050962	0.0271193882
H	-3.7112429816	-0.3261231954	-0.9996347960
H	2.9260411325	-1.1370124611	1.0802644336
P	2.5707831982	-0.3392986461	-0.0178727091
H	3.7594062586	0.3850547198	-0.1923840937
H	2.6982981218	-1.2754780020	-1.0549455721
H	0.8974853926	0.6887147288	0.0283746709
O	0.0035712917	1.2922833075	-0.0277765911
H	-0.0053354180	1.9829311160	0.6720176791

HB

H	-2.9636578662	0.8405674198	1.1400433200
P	-2.4799329500	0.1802809196	-0.0035393439
H	-2.9521878672	1.0882409753	-0.9682364246
H	-3.5023582946	-0.7779178011	-0.1208732487
H	1.7192258091	0.9965739008	1.0199053642
P	2.2908966168	0.3180515873	-0.0524118375
H	3.0201993595	-0.7586886184	0.4441507798
H	3.2381568085	1.2027731708	-0.6063922282
H	-0.3870001120	-0.5898257681	-0.0049634310
O	0.5385921324	-0.9918774523	0.0434764550
H	0.5283541486	-1.7909555527	-0.5245071086

$[\text{H}_2\text{O}-(\text{H}_2\text{S})_2]^+$

HB

H	-2.8692643909	-0.2457604069	0.7573881521
O	-2.2721124691	-0.0943711625	0.0002208041
H	-2.8710630034	0.0054791384	-0.7640306043
H	-0.5422760764	-1.3653658527	-0.1769325238
S	0.7819792151	-1.3686309910	0.0864642815
H	1.1677050715	-1.4754574481	-1.1964062578
H	-0.6633355435	1.2991366823	0.1654924864
S	0.6577645360	1.4262881456	-0.0848080246
H	1.0189467887	1.5654133840	1.2021310148

HB

H	-0.2749693106	-2.0188916642	-0.1702055566
O	-1.1264056336	-1.5846768954	0.0345995024
H	-1.8220793819	-2.2230912278	-0.2158499755
H	-1.7095260727	0.6108357252	1.2373218435
S	-1.5261624528	0.8622524362	-0.0717202095
H	-0.1565145695	0.7798733985	-0.0157478203
H	2.7339000564	0.7172643165	-0.9239885943
S	2.0257662292	0.0288747448	-0.0187592877
H	2.6887515630	0.5061733790	1.0429484031

PT

H	-0.0448488365	2.0121188120	-0.7365248087
O	-0.1599388799	1.4071025167	0.0314011867
H	-1.0139010358	0.7453419555	-0.0857140468
H	0.6794104277	0.8992642920	0.1714182073
S	2.6870938570	-0.2998734517	0.3812925742
H	3.8652627842	-0.5973038058	0.9494812319

H	-3.1722851626	-0.0119179364	-1.1833853182
S	-2.4494738818	-0.4464278549	-0.1398651451
H	-3.2501725551	0.0902896075	0.7933399935

PT

H	2.5652876361	-2.0664534026	0.5678810940
O	2.6001794126	-1.2839283690	-0.0132412086
H	3.3609527063	-1.4210323000	-0.6084207308
H	-3.3643106090	0.3386222484	-0.3908293571
S	-2.4551979000	-0.4949081393	0.1454644849
H	-0.3747125953	0.6256359378	0.0303439764
H	1.6225283650	0.0721875286	-0.0058191033
S	0.8544830936	1.2269916133	-0.0664313893
H	0.9654758915	1.5569181027	1.2321637078

[H₂O-(HCl)₂]⁺

PT

H	0.8180890239	-0.7257400596	-0.0536214319
Cl	2.4893599029	0.4058797151	0.0731468927
H	3.1498252897	0.1691760662	-1.0063588016
O	-0.0248897579	-1.2929424019	-0.0899095036
H	-0.0202932536	-1.9653492016	0.6317158601
H	-0.8563220223	-0.7278280148	-0.0402498174
Cl	-2.6614151186	0.4175633265	0.0065309777

HB

H	2.1822460792	1.4497484522	-0.8275535712
Cl	-1.3419165882	0.6787339277	0.1834125685
H	-0.2467169549	1.3924464892	0.1361764904
O	1.7305923675	1.1111532918	-0.0272122929
H	2.3022693697	1.3766233395	0.7223835893
H	1.1851290003	-0.5501331996	-0.0618293623
Cl	0.1954281883	-1.4342272509	-0.0290194939

HB

H	-0.0463571878	-0.5766575894	0.0970911235
Cl	-1.9858271037	0.1978437386	0.1885478934
H	-2.7975774835	-0.7995039647	0.2356380346
O	1.4512498195	1.3615671146	0.0253244790
H	1.9603744278	1.5800242599	-0.7912333406
H	2.0358365226	1.5803600872	0.7895725146
Cl	1.2469429082	-0.8926675513	0.0405061481