

Assessing basis set size for a calculation on H₂POH at the HF/6-31G(d,p) level.

(a)	(b)	(c)	(d)	(e)	(f)	=(c)x(d)x(e)	=(c)x(d)x(f)
Atom	AO	Degeneracy	No. Atoms	No. basis fxns per AO	No. primitives per AO	Subtotal basis functions	Subtotal primitives
H	1s (val)	1	3	2	4	6	12
	2p (pol)	3	3	1	1	9	9
O	1s (cor)	1	1	1	6	1	6
	2s (val)	1	1	2	4	2	4
	2p (val)	3	1	2	4	6	12
	3d (pol)	6	1	1	1	6	6
P	1s (cor)	1	1	1	6	1	6
	2s (cor)	1	1	1	6	1	6
	2p (cor)	3	1	1	6	3	18
	3s (val)	1	1	2	4	2	4
	3p (val)	3	1	2	4	6	12
	3d (pol)	6	1	1	1	6	6
Grand total:						49	101