Table S3 Supplementary data: X–H bond distances, X–H–Y bond distances and angles for XH + Y → X–H–Y → X + YH; distances in Å, angles in degrees

XH	R(X–H)		R(X–H)	R(H–Y)	∠ X–H–Y
H_2	H–H (0.7384)	TS3	0.8715	1.2369	173.6
		TS4	0.9873	1.1483	173.7
		TS5	1.1803	1.1226	180.0
HO_2	O–H (0.9605)	TS6	1.1324	1.2605	158.0
		TS6b	1.1046	1.2725	177.3
		TS7	1.1097	1.2984	178.1
		TS7b	1.1015	1.3155	167.2
		TS8	1.1080	1.3760	165.1
HCHO	C–H (1.0986)	TS10	1.2054	1.3764	176.3
		TS11	1.2845	1.2959	173.5
		TS12	1.3931	1.2658	174.1
H_2O	O–H (0.9502)	TS13	1.1393	1.1629	154.4
		TS13b	1.1364	1.1696	155.7
		TS14	1.2247	1.1617	158.0
		TS15	1.3704	1.1139	169.5
H_2S	S–H (1.3362)	TS16	1.4624	1.3244	164.2
		TS16b	1.4609	1.3243	162.0
		TS17	1.5488	1.2866	158.7
		TS18	1.6439	1.2168	177.4
CH_3OH	C–H (1.0832, 1.0901,1.0901)	TS19	1.2127	1.3664	160.9
		TS20	1.2885	1.2794	177.8
		TS21	1.3968	1.2568	154.6
		TS19b	1.2009	1.3745	172.1
	O–H (0.9493)	TS22	1.1348	1.2102	162.3
		TS23	1.1641	1.2211	159.9
		TS24	1.2482	1.1772	168.1
HBr	Br–H (1.4137)	TS25	1.7009	1.1977	148.6
		TS26	1.6708	1.2091	162.7
		TS27	1.7655	1.1759	180.0
HI	I–H (1.6042)	TS28	1.8067	1.3062	170.1
		TS29	1.8160	1.3479	180.0
trans-HONO	O–H (0.9549)	TS30	1.1908	1.1908	161.7
		TS31	1.1808	1.1808	180.0
		TS32	1.1535	1.2399	172.2
cis-HONO	O–H (0.9658)	TS33	1.1593	1.3148	155.9
HNO_2	N–H (1.0315)	TS34	1.1975	1.1975	180.0
		TS35	1.2318	1.2465	179.4

Notes:
YH is H-NO_2, *trans*- or *cis*-HONO.
All values obtained at BHandHLYP/6-311G(d,p) level except HI + NO_2 for which BHandHLYP/SDD values are provided.