

[supporting information]

Table S1 Molecular structures of B-series derivatives

Comp.	Structural formula	Comp.	Structural formula	Comp.	Structural formula
B ₁		B ₁₄		B ₂₇	
B ₂		B ₁₅		B ₂₈	
B ₃		B ₁₆		B ₂₉	
B ₄		B ₁₇		B ₃₀	
B ₅		B ₁₈		B ₃₁	
B ₆		B ₁₉		B ₃₂	
B ₇		B ₂₀		B ₃₃	
B ₈		B ₂₁		B ₃₄	
B ₉		B ₂₂		B ₃₅	
B ₁₀		B ₂₃			
B ₁₁		B ₂₄			

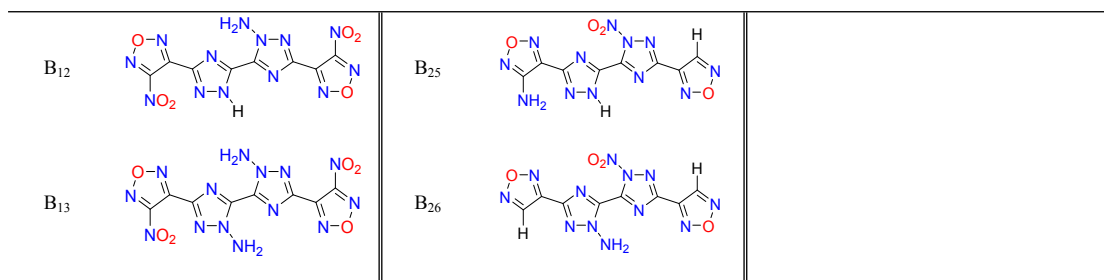


Table S2 Calculated density (ρ) and detonation properties (D, P) etc. of B-series derivatives

Comp.	ρ	D	P	HOF	h_{50}	Comp.	ρ	D	P	HOF	h_{50}
B1	1.709	6373	17.5	153.7	43	B19	1.797	7470	24.7	186.2	40
B2	1.759	6518	18.6	164.6	215	B20	1.81	7532	25.3	200.3	41
B3	1.745	6957	21.1	167.9	51	B21	1.822	7827	27.4	204.6	41
B4	1.749	6969	21.2	169.4	93	B22	1.713	6432	17.8	164.8	275
B5	1.755	6982	21.3	167.1	27	B23	1.696	6384	17.4	161.9	216
B6	1.816	7174	23	183.8	209	B24	1.735	6497	18.3	169	216
B7	1.725	6924	20.7	173.1	84	B25	1.684	6346	17.2	156.8	84
B8	1.736	6960	21	175.9	45	B26	1.7	6393	17.5	161.2	93
B9	1.755	7016	21.5	178.8	105	B27	1.743	6515	18.5	168.5	44
B10	1.761	7034	21.7	181.5	75	B28	1.724	6501	18.3	174.7	106
B11	1.771	7060	21.9	180.3	28	B29	1.707	6453	17.9	171	54
B12	1.777	7082	22.1	184.2	253	B30	1.722	6498	18.2	175.9	216
B13	1.712	6911	20.6	180.3	269	B31	1.698	6428	17.7	170.3	294
B14	1.734	6977	21.1	185.3	66	B32	1.669	6342	17	163	301
B15	1.783	7124	22.4	192.9	23	B33	1.733	6526	18.5	175.4	39
B16	1.788	7137	22.5	192.7	70	B34	1.73	6555	18.6	184.7	83
B17	1.757	7370	23.7	194.3	79	B35	1.696	6458	17.8	179.5	272
B18	1.783	7429	24.3	186.5	57						

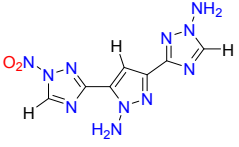
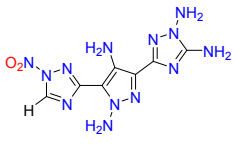
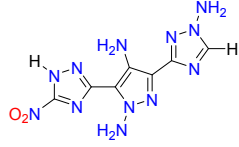
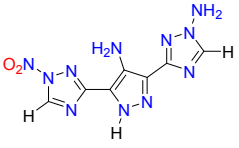
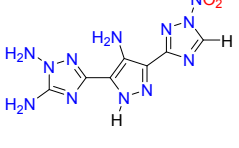
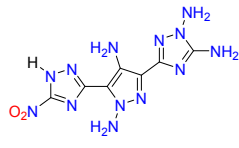
ρ (g·cm⁻³), D (m·s⁻¹), p (GPa), HOF (kJ/mol), h_{50} (cm)

Table S3 The oxygen balance (OB₁₀₀) and the nitro group charge (Q_{NO2}) of B-series derivatives

Comp.	OB ₁₀₀	Q _{NO2}	Comp.	OB ₁₀₀	Q _{NO2}	Comp.	OB ₁₀₀	Q _{NO2}	Comp.	OB ₁₀₀	Q _{NO2}
B1	-3.47	0.043	B10	-1.86	0.075	B19	-0.25	0.052	B28	-3.75	0.09
B2	-3.47	-0.139	B11	-1.86	0.03	B20	-0.47	0.052	B29	-3.75	0.054
B3	-1.66	0.057	B12	-1.86	-0.154	B21	0.88	0.056	B30	-3.75	-0.139
B4	-1.66	0.087	B13	-2.04	-0.159	B22	-3.61	-0.159	B31	-3.75	-0.165
B5	-1.66	0.029	B14	-2.04	0.068	B23	-3.61	-0.139	B32	-3.75	-0.167
B6	-1.66	-0.139	B15	-2.04	0.017	B24	-3.61	-0.139	B33	-3.75	0.037
B7	-1.86	0.081	B16	-2.04	0.071	B25	-3.61	0.077	B34	-3.87	0.076
B8	-1.86	0.051	B17	-0.47	0.081	B26	-3.61	0.083	B35	-3.87	-0.158
B9	-1.86	0.093	B18	-0.25	0.066	B27	-3.61	0.044			

Q_{NO2} (e)

Table S4 Molecular structures of D-series derivatives

Comp.	Structural formula	Comp.	Structural formula	Comp.	Structural formula
D ₁		D ₅		D ₉	
D ₂		D ₆		D ₁₀	

D ₃		D ₇		D ₁₁	
D ₄		D ₈		D ₁₂	

Continued Table S4

Comp.	Structural formula	Comp.	Structural formula	Comp.	Structural formula
D ₁₃		D ₂₃		D ₃₃	
D ₁₄		D ₂₄		D ₃₄	
D ₁₅		D ₂₅		D ₃₅	
D ₁₆		D ₂₆		D ₃₆	
D ₁₇		D ₂₇		D ₃₇	
D ₁₈		D ₂₈		D ₃₈	
D ₁₉		D ₂₉		D ₃₉	

D ₂₀		D ₃₀		D ₄₀	
D ₂₁		D ₃₁		D ₄₁	
D ₂₂		D ₃₂		D ₄₂	

Continued Table S4

Comp.	Structural formula	Comp.	Structural formula	Comp.	Structural formula
D ₄₃		D ₅₃		D ₆₃	
D ₄₄		D ₅₄		D ₆₄	
D ₄₅		D ₅₅		D ₆₅	
D ₄₆		D ₅₆		D ₆₆	
D ₄₇		D ₅₇		D ₆₇	
D ₄₈		D ₅₈		D ₆₈	

D ₄₉		D ₅₉		D ₆₉	
D ₅₀		D ₆₀		D ₇₀	
D ₅₁		D ₆₁		D ₇₁	
D ₅₂		D ₆₂		D ₇₂	

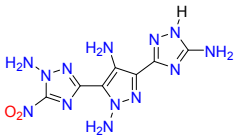
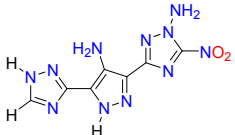
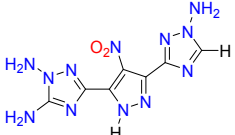
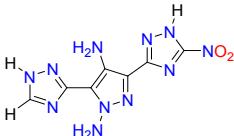
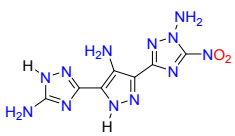
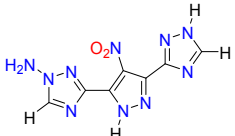
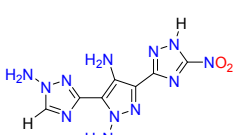
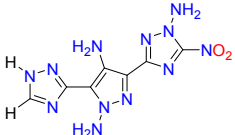
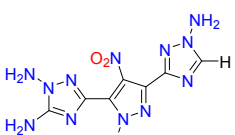
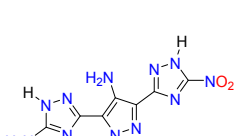
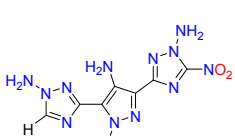
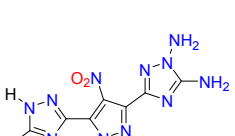
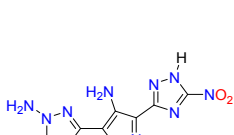
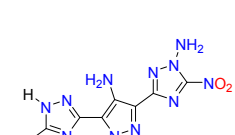
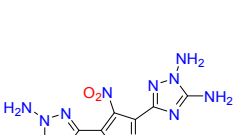
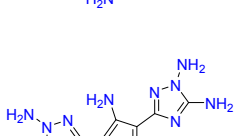
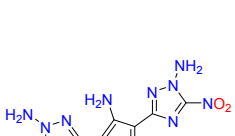
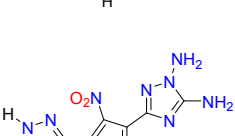
Continued Table S4

Comp.	Structural formula	Comp.	Structural formula	Comp.	Structural formula
D ₇₃		D ₈₃		D ₉₃	
D ₇₄		D ₈₄		D ₉₄	
D ₇₅		D ₈₅		D ₉₅	
D ₇₆		D ₈₆		D ₉₆	
D ₇₇		D ₈₇		D ₉₇	

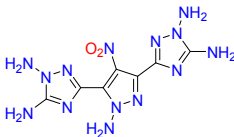
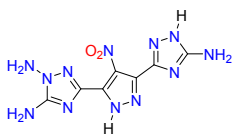
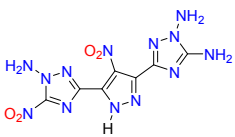
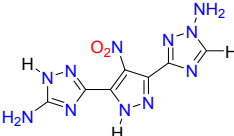
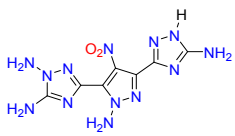
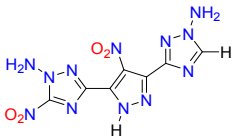
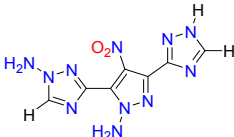
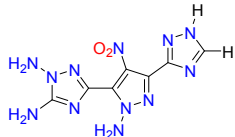
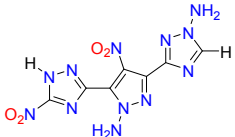
D ₇₈		D ₈₈		D ₉₈	
D ₇₉		D ₈₉		D ₉₉	
D ₈₀		D ₉₀		D ₁₀₀	
D ₈₁		D ₉₁		D ₁₀₁	
D ₈₂		D ₉₂		D ₁₀₂	

Continued Table S4

Comp.	Structural formula	Comp.	Structural formula	Comp.	Structural formula
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D ₁₀₄		D ₁₁₄		D ₁₂₄	
D ₁₀₅		D ₁₁₅		D ₁₂₅	
D ₁₀₆		D ₁₁₆		D ₁₂₆	

D ₁₀₇		D ₁₁₇		D ₁₂₇	
D ₁₀₈		D ₁₁₈		D ₁₂₈	
D ₁₀₉		D ₁₁₉		D ₁₂₉	
D ₁₁₀		D ₁₂₀		D ₁₃₀	
D ₁₁₁		D ₁₂₁		D ₁₃₁	
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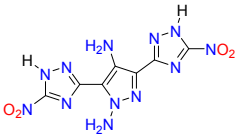
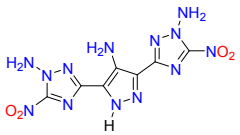
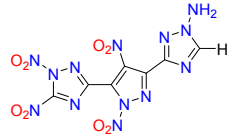
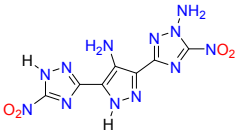
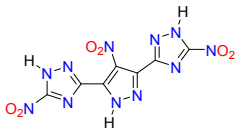
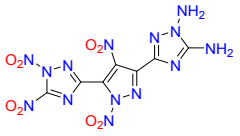
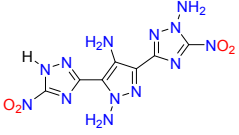
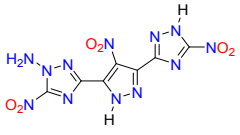
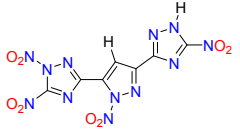
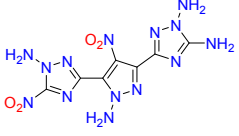
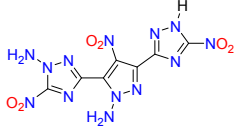
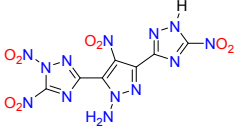
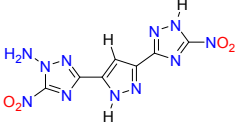
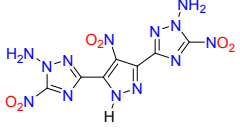
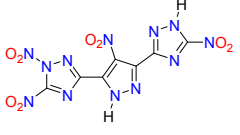
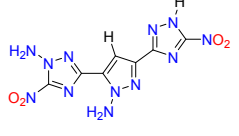
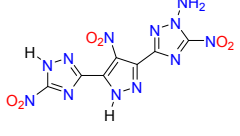
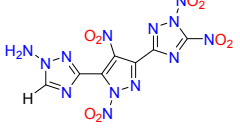
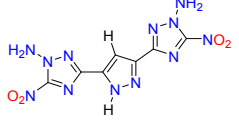
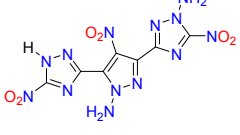
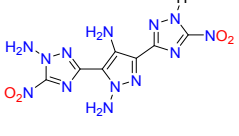
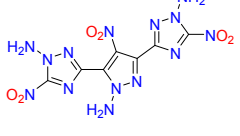
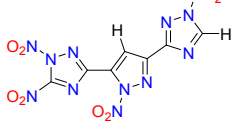
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Comp.	Structural formula	Comp.	Structural formula	Comp.	Structural formula
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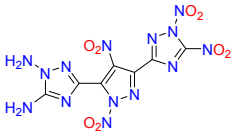
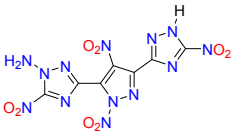
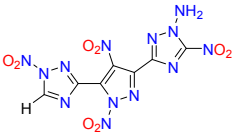
D ₁₃₆		D ₁₄₆		D ₁₅₆	
D ₁₃₇		D ₁₄₇		D ₁₅₇	
D ₁₃₈		D ₁₄₈		D ₁₅₈	
D ₁₃₉		D ₁₄₉		D ₁₅₉	
D ₁₄₀		D ₁₅₀		D ₁₆₀	
D ₁₄₁		D ₁₅₁		D ₁₆₁	
D ₁₄₂		D ₁₅₂		D ₁₆₂	

Continued Table S4

Comp.	Structural formula	Comp.	Structural formula	Comp.	Structural formula
D ₁₆₃		D ₁₇₃		D ₁₈₃	
D ₁₆₄		D ₁₇₄		D ₁₈₄	

D ₁₆₅		D ₁₇₅		D ₁₈₅	
D ₁₆₆		D ₁₇₆		D ₁₈₆	
D ₁₆₇		D ₁₇₇		D ₁₈₇	
D ₁₆₈		D ₁₇₈		D ₁₈₈	
D ₁₆₉		D ₁₇₉		D ₁₈₉	
D ₁₇₀		D ₁₈₀		D ₁₉₀	
D ₁₇₁		D ₁₈₁		D ₁₉₁	
D ₁₇₂		D ₁₈₂		D ₁₉₂	

Continued Table S4

Comp.	Structural formula	Comp.	Structural formula	Comp.	Structural formula
D ₁₉₃		D ₂₀₃		D ₂₁₃	

D ₁₉₄		D ₂₀₄		D ₂₁₄	
D ₁₉₅		D ₂₀₅		D ₂₁₅	
D ₁₉₆		D ₂₀₆		D ₂₁₆	
D ₁₉₇		D ₂₀₇		D ₂₁₇	
D ₁₉₈		D ₂₀₈		D ₂₁₈	
D ₁₉₉		D ₂₀₉		D ₂₁₉	
D ₂₀₀		D ₂₁₀		D ₂₂₀	
D ₂₀₁		D ₂₁₁		D ₂₂₁	
D ₂₀₂		D ₂₁₂		D ₂₂₂	

Continued Table S4

Comp.	Structural formula	Comp.	Structural formula	Comp.	Structural formula
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D ₂₂₃		D ₂₃₃		D ₂₄₃	
D ₂₂₄		D ₂₃₄		D ₂₄₄	
D ₂₂₅		D ₂₃₅		D ₂₄₅	
D ₂₂₆		D ₂₃₆		D ₂₄₆	
D ₂₂₇		D ₂₃₇		D ₂₄₇	
D ₂₂₈		D ₂₃₈		D ₂₄₈	
D ₂₂₉		D ₂₃₉		D ₂₄₉	
D ₂₃₀		D ₂₄₀		D ₂₅₀	
D ₂₃₁		D ₂₄₁		D ₂₅₁	
D ₂₃₂		D ₂₄₂		D ₂₅₂	

Continued Table S4

Comp.	Structural formula	Comp.	Structural formula	Comp.	Structural formula
D ₂₅₃		D ₂₆₃		D ₂₇₃	
D ₂₅₄		D ₂₆₄		D ₂₇₄	
D ₂₅₅		D ₂₆₅		D ₂₇₅	
D ₂₅₆		D ₂₆₆		D ₂₇₆	
D ₂₅₇		D ₂₆₇		D ₂₇₇	
D ₂₅₈		D ₂₆₈		D ₂₇₈	
D ₂₅₉		D ₂₆₉		D ₂₇₉	
D ₂₆₀		D ₂₇₀		D ₂₈₀	
D ₂₆₁		D ₂₇₁		D ₂₈₁	
D ₂₆₂		D ₂₇₂		D ₂₈₂	

Continued Table S4

Comp.	Structural formula	Comp.	Structural formula	Comp.	Structural formula
D ₂₈₃		D ₂₉₃		D ₃₀₃	
D ₂₈₄		D ₂₉₄		D ₃₀₄	
D ₂₈₅		D ₂₉₅		D ₃₀₅	
D ₂₈₆		D ₂₉₆		D ₃₀₆	
D ₂₈₇		D ₂₉₇		D ₃₀₇	
D ₂₈₈		D ₂₉₈		D ₃₀₈	
D ₂₈₉		D ₂₉₉		D ₃₀₉	
D ₂₉₀		D ₃₀₀		D ₃₁₀	
D ₂₉₁		D ₃₀₁		D ₃₁₁	
D ₂₉₂		D ₃₀₂		D ₃₁₂	

Continued Table S4

Comp.	Structural formula	Comp.	Structural formula	Comp.	Structural formula
D ₃₁₃		D ₃₂₃		D ₃₃₃	
D ₃₁₄		D ₃₂₄		D ₃₃₄	
D ₃₁₅		D ₃₂₅		D ₃₃₅	
D ₃₁₆		D ₃₂₆		D ₃₃₆	
D ₃₁₇		D ₃₂₇		D ₃₃₇	
D ₃₁₈		D ₃₂₈		D ₃₃₈	
D ₃₁₉		D ₃₂₉		D ₃₃₉	
D ₃₂₀		D ₃₃₀		D ₃₄₀	
D ₃₂₁		D ₃₃₁		D ₃₄₁	

D ₃₂₂		D ₃₃₂		D ₃₄₂	
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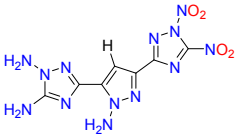
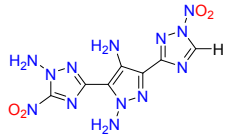
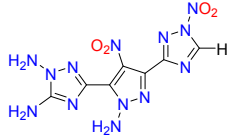
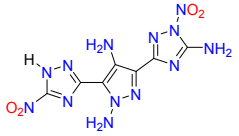
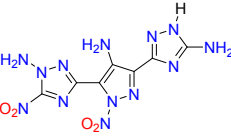
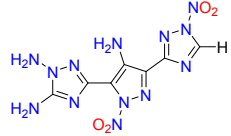
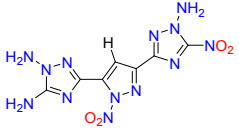
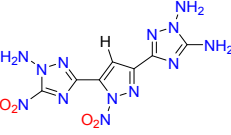
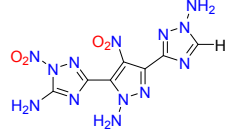
Continued Table S4

Comp.	Structural formula	Comp.	Structural formula	Comp.	Structural formula
D ₃₄₃		D ₃₅₃		D ₃₆₃	
D ₃₄₄		D ₃₅₄		D ₃₆₄	
D ₃₄₅		D ₃₅₅		D ₃₆₅	
D ₃₄₆		D ₃₅₆		D ₃₆₆	
D ₃₄₇		D ₃₅₇		D ₃₆₇	
D ₃₄₈		D ₃₅₈		D ₃₆₈	
D ₃₄₉		D ₃₅₉		D ₃₆₉	
D ₃₅₀		D ₃₆₀		D ₃₇₀	

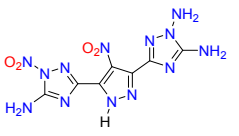
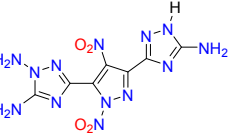
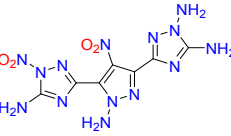
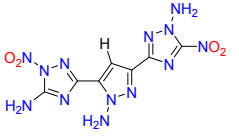
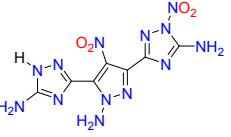
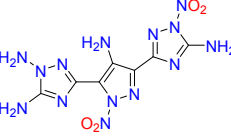
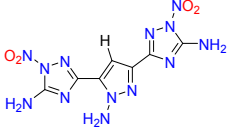
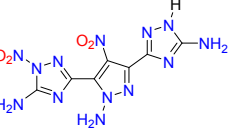
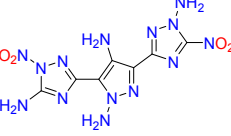
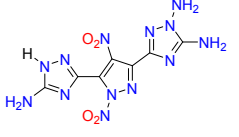
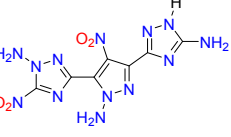
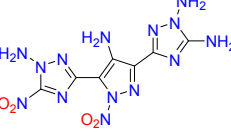
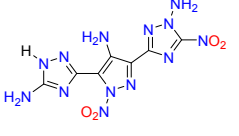
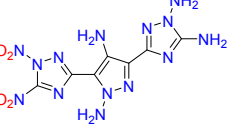
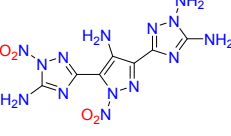
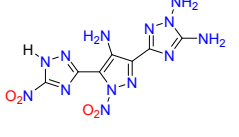
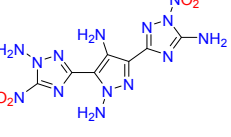
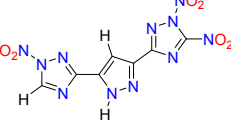
D ₃₅₁		D ₃₆₁		D ₃₇₁	
D ₃₅₂		D ₃₆₂		D ₃₇₂	

Continued Table S4

Comp.	Structural formula	Comp.	Structural formula	Comp.	Structural formula
D ₃₇₃		D ₃₈₃		D ₃₉₃	
D ₃₇₄		D ₃₈₄		D ₃₉₄	
D ₃₇₅		D ₃₈₅		D ₃₉₅	
D ₃₇₆		D ₃₈₆		D ₃₉₆	
D ₃₇₇		D ₃₈₇		D ₃₉₇	
D ₃₇₈		D ₃₈₈		D ₃₉₈	
D ₃₇₉		D ₃₈₉		D ₃₉₉	

D ₃₈₀		D ₃₉₀		D ₄₀₀	
D ₃₈₁		D ₃₉₁		D ₄₀₁	
D ₃₈₂		D ₃₉₂		D ₄₀₂	

Continued Table S4

Comp.	Structural formula	Comp.	Structural formula	Comp.	Structural formula
D ₄₀₃		D ₄₁₃		D ₄₂₃	
D ₄₀₄		D ₄₁₄		D ₄₂₄	
D ₄₀₅		D ₄₁₅		D ₄₂₅	
D ₄₀₆		D ₄₁₆		D ₄₂₆	
D ₄₀₇		D ₄₁₇		D ₄₂₇	
D ₄₀₈		D ₄₁₈		D ₄₂₈	

D ₄₀₉		D ₄₁₉		D ₄₂₉	
D ₄₁₀		D ₄₂₀		D ₄₃₀	
D ₄₁₁		D ₄₂₁		D ₄₃₁	
D ₄₁₂		D ₄₂₂		D ₄₃₂	

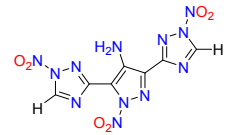
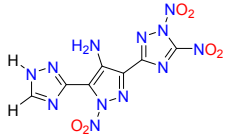
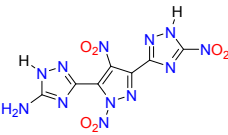
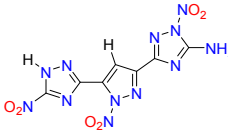
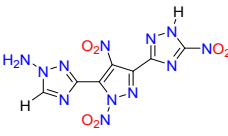
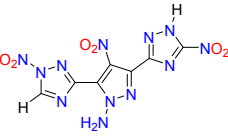
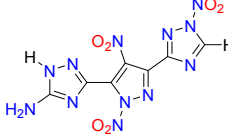
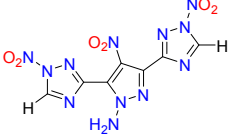
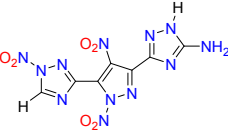
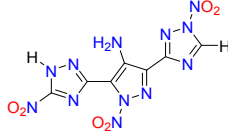
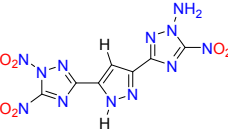
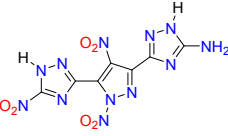
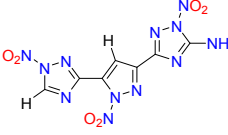
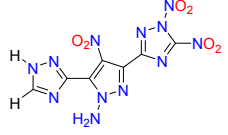
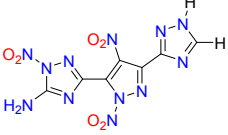
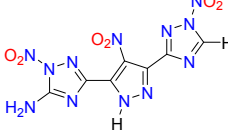
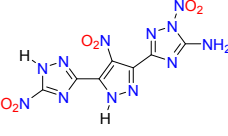
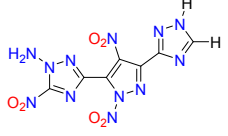
Continued Table S4

Comp.	Structural formula	Comp.	Structural formula	Comp.	Structural formula
D ₄₃₃		D ₄₄₃		D ₄₅₃	
D ₄₃₄		D ₄₄₄		D ₄₅₄	
D ₄₃₅		D ₄₄₅		D ₄₅₅	
D ₄₃₆		D ₄₄₆		D ₄₅₆	
D ₄₃₇		D ₄₄₇		D ₄₅₇	

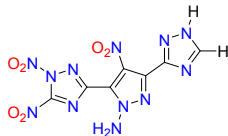
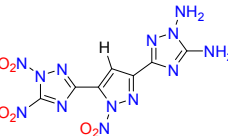
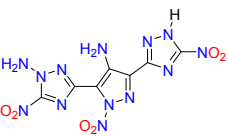
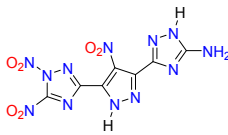
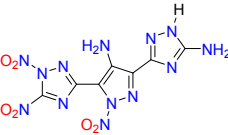
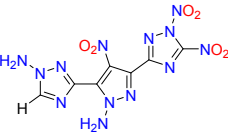
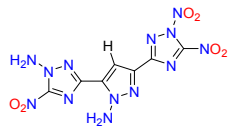
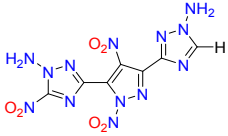
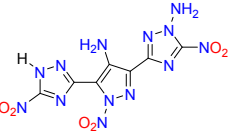
D ₄₃₈		D ₄₄₈		D ₄₅₈	
D ₄₃₉		D ₄₄₉		D ₄₅₉	
D ₄₄₀		D ₄₅₀		D ₄₆₀	
D ₄₄₁		D ₄₅₁		D ₄₆₁	
D ₄₄₂		D ₄₅₂		D ₄₆₂	

Continued Table S4

Comp.	Structural formula	Comp.	Structural formula	Comp.	Structural formula
D ₄₆₃		D ₄₇₃		D ₄₈₃	
D ₄₆₄		D ₄₇₄		D ₄₈₄	
D ₄₆₅		D ₄₇₅		D ₄₈₅	
D ₄₆₆		D ₄₇₆		D ₄₈₆	

D ₄₆₇		D ₄₇₇		D ₄₈₇	
D ₄₆₈		D ₄₇₈		D ₄₈₈	
D ₄₆₉		D ₄₇₉		D ₄₈₉	
D ₄₇₀		D ₄₈₀		D ₄₉₀	
D ₄₇₁		D ₄₈₁		D ₄₉₁	
D ₄₇₂		D ₄₈₂		D ₄₉₂	

Continued Table S4

Comp.	Structural formula	Comp.	Structural formula	Comp.	Structural formula
D ₄₉₃		D ₅₀₃		D ₅₁₃	
D ₄₉₄		D ₅₀₄		D ₅₁₄	
D ₄₉₅		D ₅₀₅		D ₅₁₅	

D ₄₉₆		D ₅₀₆		D ₅₁₆	
D ₄₉₇		D ₅₀₇		D ₅₁₇	
D ₄₉₈		D ₅₀₈		D ₅₁₈	
D ₄₉₉		D ₅₀₉		D ₅₁₉	
D ₅₀₀		D ₅₁₀		D ₅₂₀	
D ₅₀₁		D ₅₁₁		D ₅₂₁	
D ₅₀₂		D ₅₁₂		D ₅₂₂	

Continued Table S4

Comp.	Structural formula	Comp.	Structural formula	Comp.	Structural formula
D ₅₂₃		D ₅₃₃		D ₅₄₃	
D ₅₂₄		D ₅₃₄		D ₅₄₄	

D ₅₂₅		D ₅₃₅		D ₅₄₅	
D ₅₂₆		D ₅₃₆		D ₅₄₆	
D ₅₂₇		D ₅₃₇		D ₅₄₇	
D ₅₂₈		D ₅₃₈		D ₅₄₈	
D ₅₂₉		D ₅₃₉		D ₅₄₉	
D ₅₃₀		D ₅₄₀		D ₅₅₀	
D ₅₃₁		D ₅₄₁		D ₅₅₁	
D ₅₃₂		D ₅₄₂		D ₅₅₂	

Continued Table S4

Comp.	Structural formula	Comp.	Structural formula	Comp.	Structural formula
D ₅₅₃		D ₅₅₅		D ₅₅₇	

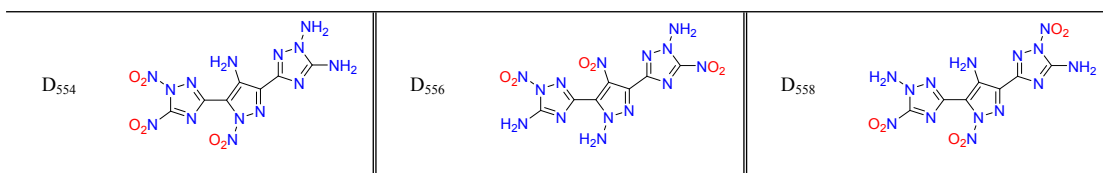


Table S5 Calculated density (ρ) and detonation properties (D, P) etc. of D-series derivatives

Comp.	ρ	D	P	HOF	h_{50}	Comp.	ρ	D	P	HOF	h_{50}
D1	1.627	5895	14.5	148.8	36	D31	1.739	6210	16.8	165	41
D2	1.636	5908	14.6	145.2	57	D32	1.658	5918	14.8	146.2	41
D3	1.616	5903	14.5	149.7	59	D33	1.695	5930	15	140.7	42
D4	1.653	6012	15.2	157.5	61	D34	1.69	6055	15.6	151	42
D5	1.631	5991	15	162.2	63	D35	1.659	5991	15.1	155.7	42
D6	1.654	6017	15.2	158	65	D36	1.717	6057	15.8	143.5	44
D7	1.635	5919	14.6	150.2	593	D37	1.701	6037	15.6	151.8	44
D8	1.646	6003	15.1	161.4	602	D38	1.667	6013	15.3	156.8	44
D9	1.636	5962	14.9	154	641	D39	1.723	6256	16.9	177.3	45
D10	1.65	6046	15.4	166	655	D40	1.665	5993	15.2	150.4	45
D11	1.643	6023	15.2	163.3	824	D41	1.687	6045	15.6	149.7	48
D12	1.65	6001	15.1	156.1	887	D42	1.657	5980	15.1	153.3	49
D13	1.651	6048	15.4	165.9	904	D43	1.715	6123	16.1	153.5	49
D14	1.721	6159	16.4	162.1	34	D44	1.717	6130	16.2	154.4	50
D15	1.691	6005	15.4	148.9	34	D45	1.679	6082	15.7	159.6	51
D16	1.725	6005	15.6	142.5	34	D46	1.712	6133	16.2	160.4	51
D17	1.663	6002	15.2	156.4	35	D47	1.699	6140	16.1	163.2	51
D18	1.694	6015	15.5	149.3	35	D48	1.738	6246	16.9	166.8	51
D19	1.704	6111	16	159.7	35	D49	1.675	6085	15.7	165.3	52
D20	1.743	6147	16.4	155.1	35	D50	1.674	6070	15.6	159.8	53
D21	1.7	6103	16	160.7	36	D51	1.722	6143	16.3	154.6	54
D22	1.665	6063	15.5	166	36	D52	1.736	6290	17.2	177.5	56
D23	1.676	6092	15.8	167.6	36	D53	1.659	6026	15.3	157.1	58
D24	1.733	6033	15.8	146.3	36	D54	1.691	6164	16.2	171.6	58
D25	1.704	6111	16	159.6	36	D55	1.696	6069	15.8	150.8	59
D26	1.723	6097	16.1	155.1	38	D56	1.681	5964	15.1	141.3	60
D27	1.7	6103	16	160.8	38	D57	1.714	6179	16.4	164.2	61
D28	1.73	6110	16.2	153.2	38	D58	1.691	6163	16.2	171.9	61
D29	1.674	6134	16	177.1	38	D59	1.718	6191	16.5	164.7	62
D30	1.708	6180	16.4	171.1	39	D60	1.689	6155	16.2	170.9	62

Continued Table S5

Comp.	ρ	D	P	HOF	h_{50}	Comp.	ρ	D	P	HOF	h_{50}
D61	1.688	6056	15.6	153	65	D103	1.735	6126	16.3	153.9	791
D62	1.745	6277	17.2	172.6	97	D104	1.706	6152	16.3	160.9	791
D63	1.748	6159	16.5	154.9	115	D105	1.743	6222	16.8	165.5	796
D64	1.663	6046	15.4	161.6	119	D106	1.7	6158	16.2	170	802
D65	1.734	6194	16.6	163.6	121	D107	1.691	6160	16.2	170.2	807
D66	1.669	6109	15.8	172.4	127	D108	1.76	6249	17.1	159.4	813
D67	1.657	5979	15.1	153.1	132	D109	1.718	6193	16.5	165.5	813
D68	1.667	6063	15.6	164.1	139	D110	1.777	6357	17.8	172.3	830
D69	1.708	6047	15.7	149.1	149	D111	1.734	6284	17.1	177.2	830
D70	1.743	6200	16.7	157.1	149	D112	1.658	6103	15.7	175.9	835
D71	1.706	6159	16.3	163.9	149	D113	1.703	6209	16.5	178.2	835
D72	1.673	6025	15.4	155.6	151	D114	1.659	6037	15.4	161.7	846
D73	1.72	6154	16.3	161.4	155	D115	1.709	6176	16.4	168.1	852
D74	1.693	6133	16.1	166.2	155	D116	1.673	6111	15.8	169.3	875
D75	1.682	6105	15.9	166.4	155	D117	1.674	6007	15.3	147.9	886
D76	1.71	6215	16.6	174	160	D118	1.677	6076	15.7	159.3	904
D77	1.713	6168	16.4	160.5	162	D119	1.672	6054	15.5	155.1	934
D78	1.76	6199	16.8	159.7	542	D120	1.656	6060	15.5	164.9	940
D79	1.76	6193	16.8	156.7	556	D121	1.702	6187	16.4	170.7	952
D80	1.668	5945	15	147.6	560	D122	1.671	6138	16	177	958
D81	1.741	6215	16.8	164.9	569	D123	1.688	6065	15.7	157.1	520
D82	1.691	6081	15.8	160.3	574	D124	1.686	6114	15.9	166.1	524
D83	1.719	6069	15.9	147.1	592	D125	1.682	6144	16.1	173.5	516
D84	1.712	6117	16.1	154.5	616	D126	1.731	6177	16.5	159	538
D85	1.658	5972	15	148.9	626	D127	1.716	6201	16.6	170.9	490
D86	1.674	6071	15.6	160.7	641	D128	1.766	6208	16.9	157.4	353
D87	1.769	6218	17	158.4	690	D129	1.708	6219	16.6	177.2	547
D88	1.754	6253	17.1	167.2	701	D130	1.749	6231	16.9	163.5	452
D89	1.758	6100	16.3	149	711	D131	1.711	6233	16.7	180	473
D90	1.71	6063	15.8	153.7	711	D132	1.732	6234	16.8	168.2	542
D91	1.77	6228	17	160.8	721	D133	1.703	6242	16.7	186.6	503
D92	1.732	6194	16.6	165.8	727	D134	1.758	6258	17.1	166.1	498
D93	1.764	6201	16.9	156.4	748	D135	1.76	6258	17.1	163.3	361
D94	1.706	6109	16	156.7	748	D136	1.828	6283	17.7	154.1	343
D95	1.722	6161	16.4	162.4	748	D137	1.749	6291	17.3	174.2	503
D96	1.749	6230	16.9	163.1	753	D138	1.769	6292	17.4	168.2	364
D97	1.676	6090	15.7	166.4	753	D139	1.758	6311	17.4	173.8	375
D98	1.785	6334	17.7	169.5	758	D140	1.823	6355	18	159.8	364
D99	1.749	6227	16.9	161.6	764	D141	1.763	6372	17.8	183.9	520

D100	1.713	6183	16.5	166.8	764	D142	1.806	6390	18.1	171.1	339
D101	1.735	6250	16.9	172.2	764	D143	1.787	6399	18.1	179.9	346
D102	1.699	6099	15.9	160.4	785	D144	1.774	6404	18	185.5	390

Continued Table S5

Comp.	ρ	D	P	HOF	h_{50}	Comp.	ρ	D	P	HOF	h_{50}
D145	1.796	6416	18.2	177	339	D187	1.823	7801	27.2	184	71
D146	1.844	6421	18.6	165.9	332	D188	1.862	7936	28.5	200.6	71
D147	1.835	6463	18.7	171.4	424	D189	1.862	7921	28.4	188.7	68
D148	1.862	6469	18.9	167.7	343	D190	1.771	7644	25.7	183.7	65
D149	1.859	6529	19.3	174.2	371	D191	1.757	7602	25.3	184.5	61
D150	1.865	6554	19.5	178.4	361	D192	1.785	7677	26	176.3	59
D151	1.848	6563	19.4	183.8	386	D193	1.774	7665	25.8	197.7	60
D152	1.779	6938	21.2	184.3	478	D194	1.818	7781	27	180	57
D153	1.741	6828	20.3	180.1	482	D195	1.776	7662	25.8	185.9	58
D154	1.737	6787	20	168.7	490	D196	1.824	7813	27.3	192.4	58
D155	1.756	6841	20.5	170.9	490	D197	1.786	7688	26.1	183.8	57
D156	1.768	6909	20.9	184.4	491	D198	1.797	7722	26.4	185.3	57
D157	1.798	6928	21.3	164.7	494	D199	1.806	7754	26.7	187.9	57
D158	1.767	6806	20.3	156.5	498	D200	1.803	7745	26.6	189.3	57
D159	1.795	6949	21.4	172.8	512	D201	1.801	7725	26.5	175.6	55
D160	1.769	6936	21.1	193.4	513	D202	1.799	7729	26.5	186.4	55
D161	1.779	6880	20.9	166.8	520	D203	1.834	7843	27.6	192.2	55
D162	1.811	7032	22	187.7	521	D204	1.829	7829	27.5	192.6	54
D163	1.767	6845	20.6	165.8	533	D205	1.844	7875	27.9	193.6	54
D164	1.744	6807	20.2	169.3	543	D206	1.786	7689	26.1	183	51
D165	1.764	6860	20.6	169.2	547	D207	1.813	7787	27	201.4	51
D166	1.72	6731	19.5	162.1	589	D208	1.793	7698	26.2	172.6	44
D167	1.706	6719	19.4	169.6	594	D209	1.779	7660	25.8	177.5	44
D168	1.737	6848	20.4	193.5	609	D210	1.787	7679	26	171.9	41
D169	1.766	6843	20.5	165.6	647	D211	1.778	7652	25.8	174.6	41
D170	1.771	6890	20.9	174.9	703	D212	1.791	7694	26.2	177.2	40
D171	1.767	6877	20.7	175.2	703	D213	1.805	7751	26.7	187.4	39
D172	1.759	6875	20.7	177.7	729	D214	1.802	7749	26.7	197.2	40
D173	1.746	6845	20.4	181.3	745	D215	1.783	7683	26	186.4	38
D174	1.704	6734	19.5	178.5	778	D216	1.798	7726	26.5	184.9	38
D175	1.721	6761	19.7	171.9	799	D217	1.809	7771	26.9	198.4	37
D176	1.824	7451	24.8	169.9	293	D218	1.807	7756	26.7	187.1	32
D177	1.814	7442	24.7	178.2	328	D219	1.79	7698	26.2	181.8	30
D178	1.811	7455	24.7	191.1	414	D220	1.796	7717	26.4	182.5	29

D179	1.798	7410	24.3	185.9	434	D221	1.79	7708	26.3	193.1	29
D180	1.796	7385	24.2	174.6	446	D222	1.794	7712	26.3	182.3	27
D181	1.795	7400	24.3	184.1	484	D223	1.791	7713	26.3	192.7	27
D182	1.797	7422	24.4	195.7	489	D224	1.775	7653	25.8	182	26
D183	1.879	7973	28.9	188.4	102	D225	1.76	7615	25.4	190.3	23
D184	1.872	7968	28.8	201.4	96	D226	1.801	7735	26.6	184	19
D185	1.784	7685	26.1	186.6	88	D227	1.801	7744	26.6	194.4	19
D186	1.791	7720	26.4	201.1	83	D228	1.818	7799	27.1	199.1	19

Continued Table S5

Comp.	ρ	D	P	HOF	h_{50}	Comp.	ρ	D	P	HOF	h_{50}
D229	1.817	8040	28.8	190.2	98	D271	1.717	6684	19.3	148.5	31
D230	1.833	8102	29.4	206.9	97	D272	1.723	6715	19.5	157.5	28
D231	1.819	8048	28.9	190.6	77	D273	1.728	6714	19.5	149.8	35
D232	1.811	8029	28.7	201.9	68	D274	1.728	6730	19.6	159	29
D233	1.835	8101	29.4	196.7	62	D275	1.729	6723	19.6	154.1	25
D234	1.823	8068	29.1	204.2	62	D276	1.729	6733	19.6	159	30
D235	1.813	8031	28.7	195	59	D277	1.73	6732	19.6	157.3	26
D236	1.819	8052	28.9	201.6	30	D278	1.734	6735	19.7	151.9	25
D237	1.878	8242	30.9	203.3	116	D279	1.735	6746	19.7	158.6	26
D238	1.842	8335	31.2	211.1	104	D280	1.739	6755	19.8	156.1	29
D239	1.71	6109	16	152.7	167	D281	1.739	6758	19.8	158.1	34
D240	1.665	6041	15.4	157.3	183	D282	1.744	6778	20	162.6	25
D241	1.691	6106	15.9	157.1	225	D283	1.744	6774	20	161.1	124
D242	1.698	6134	16.1	161.9	171	D284	1.746	6785	20	163.1	26
D243	1.7	6140	16.2	162	198	D285	1.749	6790	20.1	162.1	25
D244	1.73	6235	16.8	170.3	174	D286	1.749	6793	20.1	163.1	28
D245	1.672	6102	15.8	166.3	227	D287	1.751	6799	20.2	163.5	27
D246	1.698	6181	16.4	172.3	188	D288	1.757	6810	20.3	160.8	26
D247	1.7	6182	16.4	170.1	171	D289	1.763	6826	20.4	161.6	25
D248	1.71	6209	16.6	171	236	D290	1.765	6838	20.5	164.4	334
D249	1.664	6116	15.8	175.1	201	D291	1.765	6834	20.5	162.7	26
D250	1.686	6181	16.3	178.4	241	D292	1.769	6850	20.6	165.4	26
D251	1.709	6637	18.9	147.5	27	D293	1.775	6870	20.8	168.4	61
D252	1.728	6690	19.4	150	32	D294	1.776	6866	20.7	164	33
D253	1.737	6716	19.6	149.7	27	D295	1.779	6868	20.8	159.2	25
D254	1.74	6723	19.6	149.7	29	D296	1.784	6887	20.9	162.3	26
D255	1.743	6732	19.7	150.6	25	D297	1.79	6917	21.2	172	43
D256	1.754	6764	20	152.1	25	D298	1.795	6924	21.2	167.4	27
D257	1.762	6793	20.2	156.2	25	D299	1.805	6946	21.4	165.2	370

D258	1.785	6851	20.7	154.4	26	D300	1.817	6984	21.8	168.6	26
D259	1.798	6889	21	156.8	300	D301	1.82	6996	21.9	171.4	310
D260	1.799	6901	21.1	161.5	46	D302	1.825	7007	22	169.4	341
D261	1.818	6944	21.5	157.4	31	D303	1.833	7033	22.2	171	29
D262	1.834	6997	22	162.6	25	D304	1.834	7033	22.2	170.2	81
D263	1.841	7014	22.1	162.9	313	D305	1.838	7051	22.3	174.6	25
D264	1.698	6647	18.9	158	32	D306	1.843	7065	22.5	174.7	324
D265	1.701	6652	19	156.2	25	D307	1.846	7067	22.5	171.3	341
D266	1.702	6652	19	154.8	25	D308	1.671	6600	18.5	163.7	49
D267	1.703	6657	19	155.2	37	D309	1.699	6681	19.1	166.7	29
D268	1.71	6680	19.2	158.4	27	D310	1.702	6678	19.1	159	41
D269	1.713	6688	19.3	158.1	25	D311	1.702	6693	19.2	169.5	36
D270	1.714	6689	19.3	158.4	30	D312	1.704	6688	19.2	163.3	26

Continued Table S5

Comp.	ρ	D	P	HOF	h50	Comp.	ρ	D	P	HOF	h50
D313	1.705	6694	19.2	164.8	39	D355	1.766	6882	20.8	179.4	57
D314	1.708	6712	19.4	170.5	31	D356	1.767	6877	20.7	174.5	26
D315	1.709	6708	19.3	167.3	26	D357	1.767	6877	20.7	174.3	106
D316	1.709	6696	19.3	159.8	38	D358	1.77	6883	20.8	173.1	367
D317	1.712	6709	19.4	161.5	26	D359	1.775	6897	20.9	174	95
D318	1.716	6730	19.5	168.2	27	D360	1.779	6905	21	170.7	120
D319	1.719	6741	19.6	170.4	26	D361	1.78	6917	21.1	176.5	27
D320	1.72	6742	19.6	170.1	26	D362	1.781	6903	21	167.4	29
D321	1.721	6747	19.6	170.2	29	D363	1.785	6927	21.2	175.5	30
D322	1.721	6733	19.6	162.4	37	D364	1.786	6927	21.2	172.5	26
D323	1.724	6741	19.6	162	39	D365	1.787	6938	21.3	178.4	297
D324	1.724	6740	19.6	161.7	27	D366	1.789	6940	21.3	176.4	73
D325	1.727	6758	19.8	167.2	35	D367	1.804	6982	21.7	177.3	27
D326	1.727	6746	19.7	159	42	D368	1.813	7007	21.9	178.1	99
D327	1.729	6757	19.8	162.9	45	D369	1.825	7045	22.2	181.7	26
D328	1.729	6763	19.8	166.7	28	D370	1.827	7052	22.3	181.6	352
D329	1.73	6770	19.8	170	26	D371	1.833	7068	22.4	181.8	26
D330	1.732	6764	19.8	162.8	46	D372	1.833	7067	22.4	180.9	352
D331	1.732	6778	19.9	171.7	26	D373	1.834	7064	22.4	178	84
D332	1.733	6761	19.8	159.4	35	D374	1.837	7080	22.5	182.6	87
D333	1.734	6776	19.9	167.3	26	D375	1.843	7097	22.7	182.8	356
D334	1.735	6775	19.9	164.7	32	D376	1.695	6684	19.1	166.9	39
D335	1.735	6780	19.9	168.8	26	D377	1.706	6714	19.3	167.7	40
D336	1.735	6784	20	170	26	D378	1.707	6726	19.4	172.5	27

D337	1.736	6779	19.9	165.4	26	D379	1.708	6731	19.5	174.8	26
D338	1.736	6778	19.9	165.2	28	D380	1.71	6744	19.6	179.4	28
D339	1.737	6783	20	165.3	31	D381	1.719	6754	19.7	170.3	185
D340	1.74	6795	20.1	168.5	27	D382	1.719	6769	19.8	179.8	26
D341	1.742	6805	20.1	171.5	26	D383	1.721	6772	19.8	179.1	31
D342	1.742	6800	20.1	169.4	111	D384	1.721	6772	19.8	179.2	31
D343	1.743	6807	20.2	171.4	26	D385	1.721	6763	19.7	173.6	26
D344	1.744	6800	20.1	165.6	26	D386	1.722	6771	19.8	175.9	27
D345	1.746	6813	20.2	169.6	29	D387	1.723	6766	19.8	171.3	152
D346	1.748	6813	20.2	166.4	38	D388	1.724	6776	19.8	176.6	143
D347	1.749	6824	20.3	172	31	D389	1.725	6775	19.8	172.9	33
D348	1.751	6822	20.3	166.5	128	D390	1.725	6772	19.8	172.4	40
D349	1.752	6831	20.4	171.1	29	D391	1.731	6788	20	172.1	55
D350	1.753	6836	20.4	172.2	122	D392	1.732	6805	20.1	181.4	29
D351	1.758	6841	20.5	167.8	30	D393	1.738	6824	20.2	182	26
D352	1.759	6853	20.5	172.7	28	D394	1.738	6822	20.2	181.6	28
D353	1.76	6844	20.5	165.2	30	D395	1.739	6811	20.2	172.8	44
D354	1.762	6863	20.6	173.7	30	D396	1.741	6817	20.2	173.1	157

Continued Table S5

Comp.	ρ	D	P	HOF	h_{50}	Comp.	ρ	D	P	HOF	h_{50}
D397	1.742	6823	20.2	174.6	31	D439	1.792	7354	23.9	166.8	65
D398	1.742	6825	20.3	176.9	28	D440	1.798	7366	24	163.5	49
D399	1.747	6837	20.4	175.8	40	D441	1.818	7436	24.7	173.7	52
D400	1.75	6854	20.5	180.8	29	D442	1.823	7444	24.8	167.3	45
D401	1.753	6861	20.6	179.3	27	D443	1.828	7463	24.9	171.3	20
D402	1.754	6861	20.6	179.1	96	D444	1.841	7498	25.3	170.7	27
D403	1.754	6867	20.6	181.6	96	D445	1.846	7513	25.4	170.9	29
D404	1.756	6873	20.6	181.7	99	D446	1.884	7635	26.6	179.3	58
D405	1.758	6874	20.7	180.7	101	D447	1.74	7215	22.6	167.1	43
D406	1.762	6891	20.8	184.5	28	D448	1.74	7219	22.6	171.9	37
D407	1.762	6882	20.7	178.1	31	D449	1.741	7213	22.6	164.6	22
D408	1.771	6910	21	180.5	43	D450	1.742	7220	22.7	168.1	20
D409	1.772	6914	21	181.9	102	D451	1.743	7219	22.7	164.9	25
D410	1.775	6919	21.1	179.6	123	D452	1.743	7228	22.7	170.8	32
D411	1.777	6935	21.2	184.9	99	D453	1.744	7228	22.7	169.8	30
D412	1.781	6938	21.2	180	30	D454	1.75	7247	22.9	169.6	20
D413	1.789	6971	21.5	188.4	26	D455	1.751	7244	22.9	166.4	22
D414	1.815	7039	22.1	186.7	108	D456	1.752	7252	22.9	169.7	30
D415	1.832	7091	22.5	189.9	89	D457	1.754	7250	23	163.5	19

D416	1.855	7160	23.2	194.2	339	D458	1.756	7255	23	163.2	25
D417	1.682	6677	19	180.1	27	D459	1.758	7272	23.1	171.3	21
D418	1.716	6770	19.7	180.2	173	D460	1.759	7272	23.1	170.4	31
D419	1.719	6787	19.9	185.4	29	D461	1.76	7282	23.2	174.5	35
D420	1.727	6801	20	179.8	157	D462	1.761	7269	23.1	164.1	19
D421	1.728	6818	20.1	191.3	29	D463	1.761	7279	23.2	170.9	22
D422	1.741	6847	20.4	186.7	30	D464	1.763	7287	23.3	171.8	50
D423	1.745	6863	20.5	188.9	103	D465	1.766	7290	23.3	169	19
D424	1.754	6885	20.7	188	29	D466	1.766	7299	23.4	174.4	38
D425	1.757	6890	20.8	186.1	157	D467	1.768	7294	23.3	166.5	19
D426	1.76	6903	20.9	188.7	52	D468	1.768	7301	23.4	172.1	20
D427	1.784	6972	21.4	191.6	39	D469	1.776	7324	23.6	173.1	41
D428	1.737	7187	22.4	159.1	32	D470	1.778	7323	23.6	167.7	19
D429	1.744	7206	22.6	160	32	D471	1.779	7336	23.7	174.4	22
D430	1.746	7210	22.6	158.6	22	D472	1.78	7335	23.7	171.4	19
D431	1.753	7236	22.9	162.5	41	D473	1.783	7348	23.8	175.5	22
D432	1.759	7250	23	160.7	23	D474	1.783	7341	23.8	169.9	37
D433	1.761	7256	23	161	36	D475	1.783	7346	23.8	174.6	24
D434	1.774	7291	23.4	159.1	40	D476	1.786	7351	23.9	171.3	35
D435	1.776	7304	23.5	164.2	25	D477	1.787	7352	23.9	169.6	26
D436	1.778	7307	23.5	160.9	18	D478	1.791	7371	24	176.3	48
D437	1.778	7310	23.5	164.3	26	D479	1.791	7371	24	173.9	19
D438	1.784	7325	23.7	163	18	D480	1.791	7375	24.1	179.8	41

Continued Table S5

Comp.	ρ	D	P	HOF	h_{50}	Comp.	ρ	D	P	HOF	h_{50}
D481	1.792	7371	24	172.1	43	D520	1.767	7316	23.5	182.1	28
D482	1.793	7374	24.1	173	76	D521	1.768	7321	23.5	184	27
D483	1.795	7386	24.2	179	51	D522	1.774	7332	23.6	177.8	20
D484	1.8	7401	24.3	177.9	46	D523	1.774	7330	23.6	177	20
D485	1.806	7422	24.5	182.2	76	D524	1.779	7345	23.8	177.8	19
D486	1.821	7461	24.9	179.1	60	D525	1.782	7355	23.9	178	22
D487	1.83	7491	25.1	181.5	39	D526	1.783	7370	24	188	47
D488	1.833	7498	25.2	180.7	20	D527	1.783	7361	23.9	181.8	78
D489	1.839	7520	25.4	183.2	24	D528	1.787	7377	24	184.3	35
D490	1.842	7527	25.5	183.1	22	D529	1.787	7375	24	183	69
D491	1.849	7547	25.7	181.1	25	D530	1.79	7383	24.1	183.8	25
D492	1.853	7558	25.8	182.3	23	D531	1.791	7388	24.1	185.8	21
D493	1.88	7645	26.6	189.2	63	D532	1.795	7409	24.3	190.8	46
D494	1.887	7670	26.8	192.5	54	D533	1.795	7401	24.3	186.5	32

D495	1.729	7201	22.4	178.1	26	D534	1.796	7404	24.3	184.8	20
D496	1.731	7200	22.5	172.5	20	D535	1.798	7410	24.3	185.4	20
D497	1.734	7212	22.6	173.7	24	D536	1.802	7424	24.5	187.5	41
D498	1.74	7228	22.7	175	23	D537	1.828	7504	25.2	191.4	25
D499	1.741	7244	22.8	184.2	35	D538	1.849	7568	25.8	194.2	20
D500	1.744	7247	22.9	179.8	27	D539	1.882	7673	26.8	201	53
D501	1.748	7253	22.9	176.7	22	D540	1.722	7189	22.3	182.2	23
D502	1.75	7260	23	175.8	23	D541	1.732	7218	22.6	183.2	23
D503	1.752	7276	23.1	185.8	47	D542	1.734	7224	22.6	184.3	20
D504	1.753	7270	23.1	176.5	23	D543	1.745	7258	22.9	184.7	20
D505	1.753	7272	23.1	179.9	35	D544	1.759	7297	23.3	185.3	27
D506	1.753	7275	23.1	181.9	36	D545	1.764	7324	23.5	194.2	31
D507	1.754	7270	23.1	176.7	21	D546	1.765	7325	23.5	193.5	34
D508	1.755	7277	23.1	178.5	28	D547	1.769	7337	23.6	193.5	27
D509	1.755	7272	23.1	174.3	20	D548	1.77	7347	23.7	199.2	53
D510	1.756	7284	23.2	181	39	D549	1.77	7344	23.7	195.3	29
D511	1.757	7277	23.1	173.4	19	D550	1.772	7343	23.7	191.1	83
D512	1.758	7286	23.2	180.1	39	D551	1.776	7361	23.8	196.1	40
D513	1.759	7283	23.2	174.5	20	D552	1.78	7372	23.9	196.2	24
D514	1.76	7295	23.3	181.1	44	D553	1.786	7381	24.1	188.6	22
D515	1.762	7291	23.3	175	22	D554	1.799	7430	24.5	197.6	21
D516	1.763	7305	23.4	183.5	26	D555	1.799	7422	24.4	192.1	21
D517	1.763	7308	23.4	186.1	52	D556	1.806	7446	24.6	195.9	48
D518	1.763	7307	23.4	184.8	50	D557	1.821	7493	25.1	197.5	50
D519	1.765	7308	23.4	179.7	21	D558	1.778	7357	23.8	188	26

ρ ($\text{g}\cdot\text{cm}^{-3}$), D ($\text{m}\cdot\text{s}^{-1}$), P (GPa), HOF (kJ/mol), h_{50} (cm)

Table S6 The oxygen balance (OB_{100}) and the nitro group charge (Q_{NO_2}) of D-series derivatives

Comp.	OB_{100}	Q_{NO_2}	Comp.	OB_{100}	Q_{NO_2}	Comp.	OB_{100}	Q_{NO_2}	Comp.	OB_{100}	Q_{NO_2}
D1	-6.14	-0.016	D43	-6.14	-0.039	D85	-6.14	-0.245	D127	-6.16	-0.215
D2	-6.14	-0.048	D44	-6.14	-0.04	D86	-6.16	-0.248	D128	-6.11	-0.18
D3	-6.16	-0.05	D45	-6.16	-0.042	D87	-6.11	-0.258	D129	-6.19	-0.228
D4	-6.16	-0.052	D46	-6.14	-0.042	D88	-6.14	-0.26	D130	-6.14	-0.206
D5	-6.19	-0.054	D47	-6.16	-0.042	D89	-6.07	-0.262	D131	-6.19	-0.211
D6	-6.16	-0.056	D48	-6.16	-0.042	D90	-6.11	-0.262	D132	-6.16	-0.227
D7	-6.14	-0.238	D49	-6.16	-0.043	D91	-6.11	-0.264	D133	-6.21	-0.218
D8	-6.16	-0.24	D50	-6.16	-0.044	D92	-6.14	-0.265	D134	-6.14	-0.217

D9	-6.16	-0.248	D51	-6.14	-0.045	D93	-6.11	-0.269	D135	-6.14	-0.182
D10	-6.19	-0.251	D52	-6.19	-0.047	D94	-6.14	-0.269	D136	-6.07	-0.177
D11	-6.19	-0.283	D53	-6.16	-0.049	D95	-6.14	-0.269	D137	-6.16	-0.218
D12	-6.16	-0.294	D54	-6.19	-0.049	D96	-6.14	-0.27	D138	-6.14	-0.183
D13	-6.19	-0.297	D55	-6.14	-0.05	D97	-6.16	-0.27	D139	-6.16	-0.186
D14	-6.14	-0.002	D56	-6.11	-0.052	D98	-6.14	-0.271	D140	-6.11	-0.183
D15	-6.11	-0.006	D57	-6.16	-0.052	D99	-6.14	-0.272	D141	-6.19	-0.222
D16	-6.07	-0.007	D58	-6.19	-0.052	D100	-6.16	-0.272	D142	-6.14	-0.176
D17	-6.14	-0.009	D59	-6.16	-0.053	D101	-6.16	-0.272	D143	-6.16	-0.178
D18	-6.11	-0.01	D60	-6.19	-0.053	D102	-6.14	-0.276	D144	-6.19	-0.19
D19	-6.14	-0.012	D61	-6.14	-0.056	D103	-6.11	-0.277	D145	-6.16	-0.176
D20	-6.11	-0.013	D62	-6.16	-0.08	D104	-6.16	-0.277	D146	-6.11	-0.174
D21	-6.14	-0.015	D63	-6.11	-0.091	D105	-6.14	-0.278	D147	-6.14	-0.199
D22	-6.16	-0.015	D64	-6.16	-0.093	D106	-6.16	-0.279	D148	-6.11	-0.177
D23	-6.16	-0.015	D65	-6.14	-0.094	D107	-6.19	-0.28	D149	-6.14	-0.185
D24	-6.07	-0.016	D66	-6.19	-0.097	D108	-6.14	-0.281	D150	-6.14	-0.182
D25	-6.14	-0.016	D67	-6.14	-0.1	D109	-6.16	-0.281	D151	-6.16	-0.189
D26	-6.11	-0.02	D68	-6.16	-0.103	D110	-6.16	-0.284	D152	-3.86	-0.214
D27	-6.14	-0.02	D69	-6.11	-0.108	D111	-6.19	-0.284	D153	-3.86	-0.215
D28	-6.11	-0.021	D70	-6.14	-0.108	D112	-6.21	-0.285	D154	-3.73	-0.217
D29	-6.19	-0.021	D71	-6.16	-0.108	D113	-6.19	-0.285	D155	-3.73	-0.217
D30	-6.16	-0.022	D72	-6.14	-0.109	D114	-6.16	-0.287	D156	-3.86	-0.217
D31	-6.14	-0.026	D73	-6.14	-0.111	D115	-6.16	-0.288	D157	-3.58	-0.218
D32	-6.11	-0.028	D74	-6.16	-0.111	D116	-6.19	-0.292	D158	-3.42	-0.219
D33	-6.07	-0.029	D75	-6.16	-0.111	D117	-6.14	-0.294	D159	-3.73	-0.222
D34	-6.14	-0.029	D76	-6.19	-0.113	D118	-6.16	-0.297	D160	-3.98	-0.222
D35	-6.14	-0.029	D77	-6.16	-0.114	D119	-6.16	-0.302	D161	-3.58	-0.224
D36	-6.11	-0.032	D78	-6.11	-0.227	D120	-6.19	-0.303	D162	-3.86	-0.224
D37	-6.11	-0.032	D79	-6.11	-0.23	D121	-6.19	-0.305	D163	-3.58	-0.227
D38	-6.14	-0.032	D80	-6.11	-0.231	D122	-6.21	-0.306	D164	-3.73	-0.229
D39	-6.19	-0.033	D81	-6.14	-0.233	D123	-6.14	-0.222	D165	-3.73	-0.23
D40	-6.14	-0.034	D82	-6.14	-0.234	D124	-6.16	-0.223	D166	-3.73	-0.239
D41	-6.14	-0.038	D83	-6.11	-0.238	D125	-6.19	-0.221	D167	-3.86	-0.24
D42	-6.14	-0.039	D84	-6.14	-0.243	D126	-6.14	-0.226	D168	-3.98	-0.243

Continued Table S6

Comp.	OB ₁₀₀	Q _{NO2}	Comp.	OB ₁₀₀	Q _{NO2}	Comp.	OB ₁₀₀	Q _{NO2}	Comp.	OB ₁₀₀	Q _{NO2}
D169	-3.58	-0.251	D211	0.00	0.053	D253	-3.42	0.014	D295	-3.58	-0.005
D170	-3.73	-0.262	D212	0.00	0.052	D254	-3.42	0.022	D296	-3.58	-0.01
D171	-3.73	-0.262	D213	-0.25	0.051	D255	-3.42	0.006	D297	-3.58	0.043

D172	-3.86	-0.267	D214	-0.49	0.051	D256	-3.42	0.001	D298	-3.58	-0.013
D173	-3.86	-0.27	D215	-0.25	0.05	D257	-3.42	-0.004	D299	-3.58	-0.187
D174	-3.98	-0.276	D216	-0.25	0.049	D258	-3.42	-0.01	D300	-3.58	0.011
D175	-3.86	-0.28	D217	-0.49	0.048	D259	-3.42	-0.167	D301	-3.58	-0.17
D176	-1.48	-0.167	D218	-0.25	0.043	D260	-3.42	0.047	D302	-3.58	-0.179
D177	-1.70	-0.177	D219	-0.25	0.041	D261	-3.42	0.025	D303	-3.58	0.019
D178	-1.91	-0.2	D220	-0.25	0.039	D262	-3.42	0.002	D304	-3.58	-0.075
D179	-1.91	-0.205	D221	-0.49	0.038	D263	-3.42	-0.171	D305	-3.58	-0.001
D180	-1.70	-0.208	D222	-0.25	0.036	D264	-3.58	0.026	D306	-3.58	-0.174
D181	-1.91	-0.217	D223	-0.49	0.036	D265	-3.58	-0.003	D307	-3.58	-0.179
D182	-2.09	-0.218	D224	-0.25	0.035	D266	-3.58	-0.005	D308	-3.73	0.049
D183	0.00	0.095	D225	-0.49	0.029	D267	-3.58	-0.034	D309	-3.73	0.017
D184	-0.25	0.091	D226	-0.25	0.024	D268	-3.58	0.015	D310	-3.73	-0.04
D185	-0.25	0.087	D227	-0.49	0.021	D269	-3.58	-0.001	D311	-3.73	0.033
D186	-0.49	0.083	D228	-0.49	0.021	D270	-3.58	0.023	D312	-3.73	0.006
D187	0.00	0.077	D229	1.17	0.095	D271	-3.58	-0.024	D313	-3.73	-0.037
D188	-0.25	0.076	D230	0.90	0.094	D272	-3.58	0.018	D314	-3.73	0.024
D189	0.00	0.075	D231	1.17	0.083	D273	-3.58	-0.032	D315	-3.73	0.008
D190	-0.25	0.072	D232	0.90	0.077	D274	-3.58	-0.019	D316	-3.73	-0.035
D191	-0.25	0.069	D233	1.17	0.073	D275	-3.58	0.005	D317	-3.73	0.003
D192	0.00	0.068	D234	0.90	0.073	D276	-3.58	-0.021	D318	-3.73	-0.011
D193	-0.49	0.068	D235	1.17	0.071	D277	-3.58	0.007	D319	-3.73	0.009
D194	0.00	0.067	D236	0.90	0.045	D278	-3.58	0	D320	-3.73	-0.007
D195	-0.25	0.067	D237	1.17	0.104	D279	-3.58	-0.01	D321	-3.73	0.017
D196	-0.25	0.067	D238	2.12	0.1	D280	-3.58	0.019	D322	-3.73	-0.034
D197	-0.25	0.066	D239	-6.14	-0.116	D281	-3.58	0.03	D323	-3.73	-0.037
D198	-0.25	0.066	D240	-6.16	-0.123	D282	-3.58	0.001	D324	-3.73	-0.01
D199	-0.25	0.066	D241	-6.16	-0.139	D283	-3.58	-0.1	D325	-3.73	-0.031
D200	-0.25	0.066	D242	-6.16	-0.118	D284	-3.58	0.008	D326	-3.73	-0.041
D201	0.00	0.065	D243	-6.16	-0.129	D285	-3.58	-0.004	D327	-3.73	-0.044
D202	-0.25	0.065	D244	-6.16	-0.119	D286	-3.58	0.016	D328	-3.73	0.014
D203	-0.25	0.065	D245	-6.19	-0.14	D287	-3.58	-0.015	D329	-3.73	0.007
D204	-0.25	0.064	D246	-6.19	-0.125	D288	-3.58	0.006	D330	-3.73	-0.045
D205	-0.25	0.064	D247	-6.19	-0.118	D289	-3.58	-0.005	D331	-3.73	-0.008
D206	-0.25	0.061	D248	-6.19	-0.143	D290	-3.58	-0.177	D332	-3.73	-0.03
D207	-0.49	0.061	D249	-6.21	-0.13	D291	-3.58	-0.009	D333	-3.73	0.001
D208	0.00	0.056	D250	-6.21	-0.145	D292	-3.58	0.011	D334	-3.73	-0.026
D209	0.00	0.056	D251	-3.42	-0.015	D293	-3.58	0.06	D335	-3.73	-0.009
D210	0.00	0.053	D252	-3.42	0.027	D294	-3.58	0.028	D336	-3.73	-0.008

Continued Table S6

Comp.	OB ₁₀₀	Q _{NO2}	Comp.	OB ₁₀₀	Q _{NO2}	Comp.	OB ₁₀₀	Q _{NO2}	Comp.	OB ₁₀₀	Q _{NO2}
D337	-3.73	-0.005	D379	-3.86	0.001	D421	-3.98	0.015	D463	-1.70	0.018
D338	-3.73	0.016	D380	-3.86	0.013	D422	-3.98	-0.019	D464	-1.70	0.056
D339	-3.73	-0.024	D381	-3.86	-0.127	D423	-3.98	-0.088	D465	-1.70	-0.002
D340	-3.73	-0.01	D382	-3.86	0.002	D424	-3.98	-0.017	D466	-1.70	0.044
D341	-3.73	0.001	D383	-3.86	0.022	D425	-3.98	-0.115	D467	-1.70	0.006
D342	-3.73	-0.093	D384	-3.86	0.022	D426	-3.98	-0.051	D468	-1.70	0.012
D343	-3.73	-0.008	D385	-3.86	-0.004	D427	-3.98	-0.036	D469	-1.70	0.048
D344	-3.73	-0.007	D386	-3.86	0.008	D428	-1.48	0.037	D470	-1.70	0.006
D345	-3.73	0.019	D387	-3.86	-0.113	D429	-1.48	0.038	D471	-1.70	0.018
D346	-3.73	-0.035	D388	-3.86	-0.109	D430	-1.48	0.019	D472	-1.70	-0.004
D347	-3.73	0.024	D389	-3.86	-0.026	D431	-1.48	0.048	D473	-1.70	0.019
D348	-3.73	-0.102	D390	-3.86	-0.037	D432	-1.48	0.023	D474	-1.70	0.043
D349	-3.73	0.018	D391	-3.86	-0.054	D433	-1.48	0.043	D475	-1.70	0.023
D350	-3.73	-0.099	D392	-3.86	-0.018	D434	-1.48	0.047	D476	-1.70	0.04
D351	-3.73	-0.02	D393	-3.86	0.001	D435	-1.48	0.027	D477	-1.70	0.028
D352	-3.73	-0.014	D394	-3.86	-0.013	D436	-1.48	-0.001	D478	-1.70	0.054
D353	-3.73	-0.022	D395	-3.86	-0.043	D437	-1.48	0.029	D479	-1.70	0.004
D354	-3.73	-0.02	D396	-3.86	-0.115	D438	-1.48	0.005	D480	-1.70	0.048
D355	-3.73	0.056	D397	-3.86	-0.023	D439	-1.48	0.069	D481	-1.70	0.05
D356	-3.73	0	D398	-3.86	-0.015	D440	-1.48	0.056	D482	-1.70	-0.076
D357	-3.73	-0.09	D399	-3.86	-0.038	D441	-1.48	0.059	D483	-1.70	0.057
D358	-3.73	-0.186	D400	-3.86	-0.018	D442	-1.48	0.052	D484	-1.70	0.053
D359	-3.73	-0.084	D401	-3.86	-0.009	D443	-1.48	0.013	D485	-1.70	0.076
D360	-3.73	-0.098	D402	-3.86	-0.084	D444	-1.48	0.031	D486	-1.70	-0.065
D361	-3.73	0.013	D403	-3.86	-0.084	D445	-1.48	0.034	D487	-1.70	0.045
D362	-3.73	-0.019	D404	-3.86	-0.086	D446	-1.48	0.064	D488	-1.70	0.01
D363	-3.73	0.021	D405	-3.86	-0.087	D447	-1.70	0.05	D489	-1.70	0.023
D364	-3.73	-0.008	D406	-3.86	0.013	D448	-1.70	0.043	D490	-1.70	0.017
D365	-3.73	-0.166	D407	-3.86	-0.022	D449	-1.70	0.017	D491	-1.70	0.026
D366	-3.73	-0.069	D408	-3.86	-0.042	D450	-1.70	0.012	D492	-1.70	0.021
D367	-3.73	-0.013	D409	-3.86	-0.088	D451	-1.70	0.025	D493	-1.70	0.067
D368	-3.73	-0.086	D410	-3.86	-0.099	D452	-1.70	0.037	D494	-1.70	0.06
D369	-3.73	0.008	D411	-3.86	-0.086	D453	-1.70	0.033	D495	-1.91	0.026
D370	-3.73	-0.182	D412	-3.86	-0.019	D454	-1.70	0.013	D496	-1.91	0.003
D371	-3.73	0	D413	-3.86	0.006	D455	-1.70	0.018	D497	-1.91	0.021
D372	-3.73	-0.182	D414	-3.86	-0.091	D456	-1.70	0.033	D498	-1.91	0.019
D373	-3.73	-0.077	D415	-3.86	-0.08	D457	-1.70	0.006	D499	-1.91	0.04
D374	-3.73	-0.079	D416	-3.86	-0.178	D458	-1.70	0.025	D500	-1.91	0.027
D375	-3.73	-0.183	D417	-3.98	0	D459	-1.70	0.014	D501	-1.91	0.015

D376	-3.86	-0.036	D418	-3.98	-0.122	D460	-1.70	0.035	D502	-1.91	0.019
D377	-3.86	-0.038	D419	-3.98	-0.017	D461	-1.70	0.041	D503	-1.91	0.053
D378	-3.86	-0.011	D420	-3.98	-0.115	D462	-1.70	-0.001	D504	-1.91	0.019

Continued Table S6

Comp.	OB ₁₀₀	Q _{NO2}	Comp.	OB ₁₀₀	Q _{NO2}	Comp.	OB ₁₀₀	Q _{NO2}	Comp.	OB ₁₀₀	Q _{NO2}
D505	-1.91	0.04	D519	-1.91	0.013	D533	-1.91	0.035	D547	-2.09	0.026
D506	-1.91	0.041	D520	-1.91	0.029	D534	-1.91	0.003	D548	-2.09	0.058
D507	-1.91	0.013	D521	-1.91	0.027	D535	-1.91	-0.007	D549	-2.09	0.03
D508	-1.91	0.029	D522	-1.91	0.004	D536	-1.91	0.047	D550	-2.09	-0.08
D509	-1.91	-0.009	D523	-1.91	-0.007	D537	-1.91	0.023	D551	-2.09	0.045
D510	-1.91	0.044	D524	-1.91	0.002	D538	-1.91	0.01	D552	-2.09	0.02
D511	-1.91	0.001	D525	-1.91	-0.015	D539	-1.91	0.058	D553	-2.09	-0.012
D512	-1.91	0.045	D526	-1.91	0.053	D540	-2.09	0.017	D554	-2.09	0.009
D513	-1.91	-0.01	D527	-1.91	-0.077	D541	-2.09	0.016	D555	-2.09	-0.007
D514	-1.91	0.05	D528	-1.91	0.04	D542	-2.09	-0.001	D556	-2.09	-0.053
D515	-1.91	-0.017	D529	-1.91	-0.071	D543	-2.09	-0.003	D557	-2.09	-0.055
D516	-1.91	0.025	D530	-1.91	0.024	D544	-2.09	-0.026	D558	-2.09	-0.024
D517	-1.91	0.057	D531	-1.91	0.014	D545	-2.09	0.033			
D518	-1.91	0.056	D532	-1.91	0.052	D546	-2.09	0.038			

Q_{NO2} (e)

According to the above information, in the B series, the compound having a detonation velocity greater than that of TNT contains at least two -NO₂ groups, and the compound having a detonation velocity less than or equal to that of TNT contains at most two -NO₂ groups and at least one -NO₂ group. In the D series, the compound having a detonation velocity greater than that of TNT contains at least two -NO₂ groups, and the compound having a detonation velocity less than or equal to that of TNT contains at most two -NO₂ groups. However, the detonation velocity of compounds containing one -NO₂ group in the D series is less than that of TNT.