Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Ab initio calculations and QTAIM analyses of the structure and energetics of hydrated calcium fluoride and calcium carbonate

SUPPLEMENTARY MATERIAL

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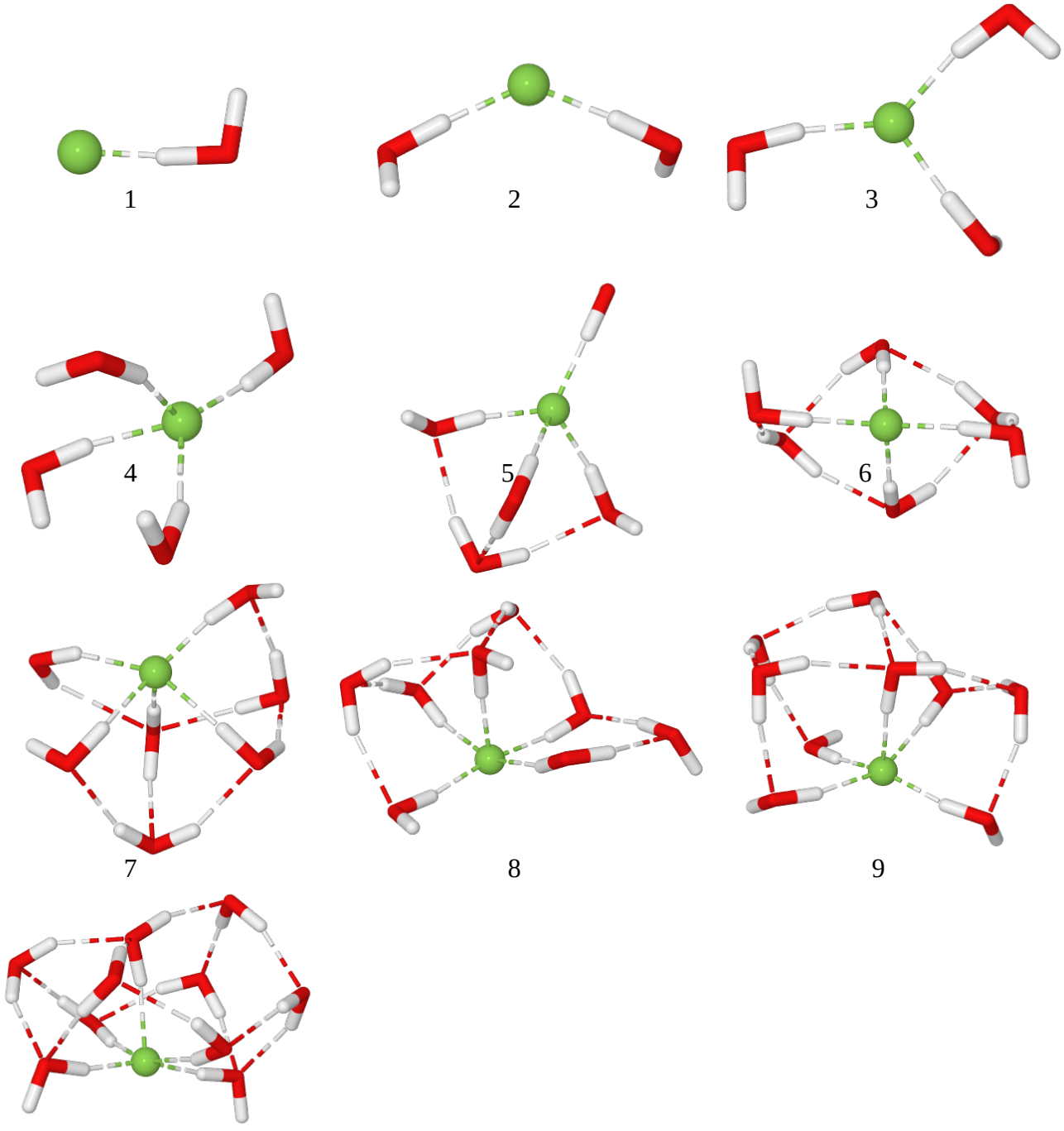

Fig. S1. Optimum structures for $F^{-}(H_2O)_n$, n = 1–10, calculated using MP2/6-311++G**.

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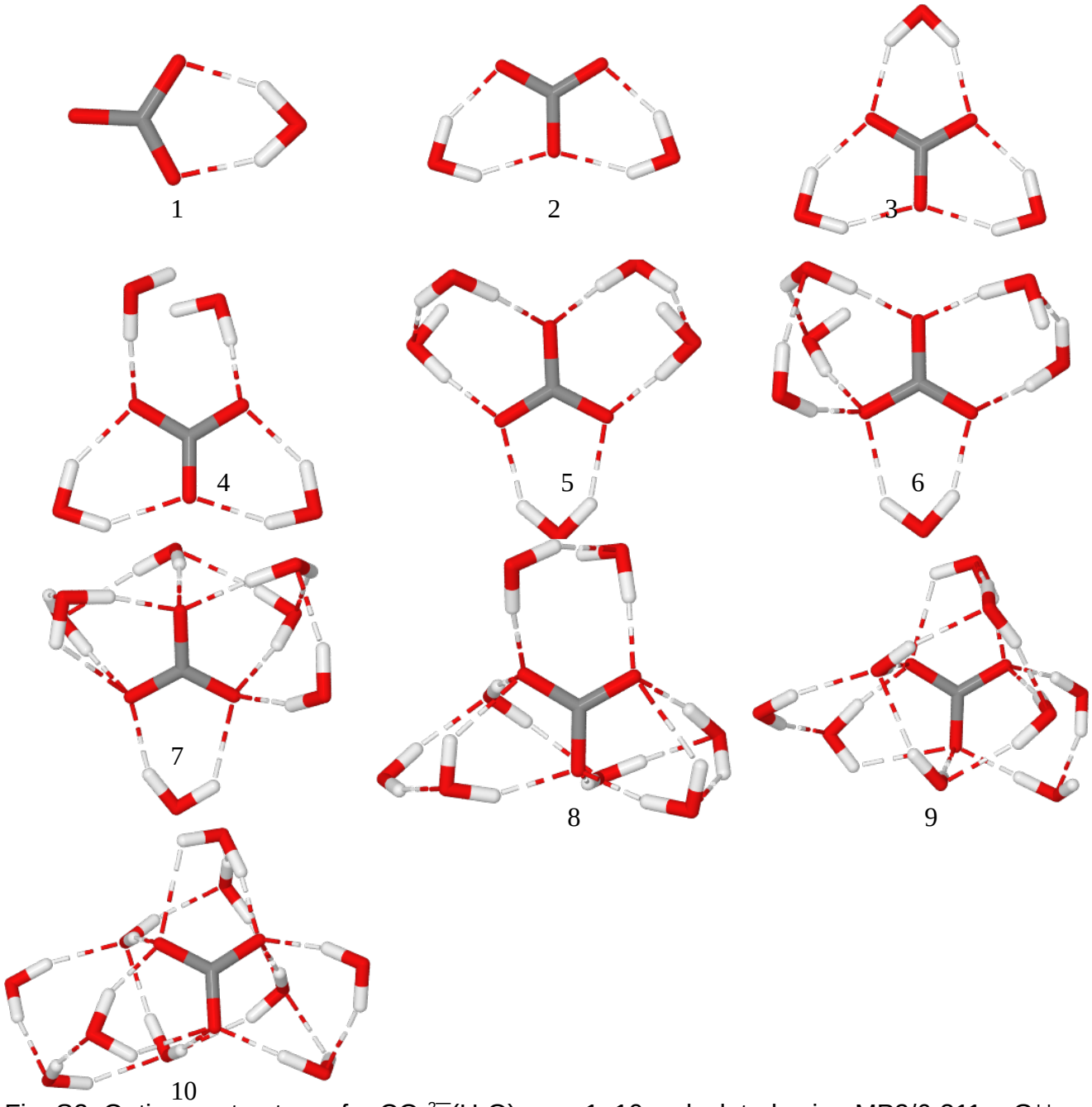

Fig. S2. Optimum structures for $CO_3^{2-}(H_2O)_n$, n = 1–10, calculated using MP2/6-311++G**.

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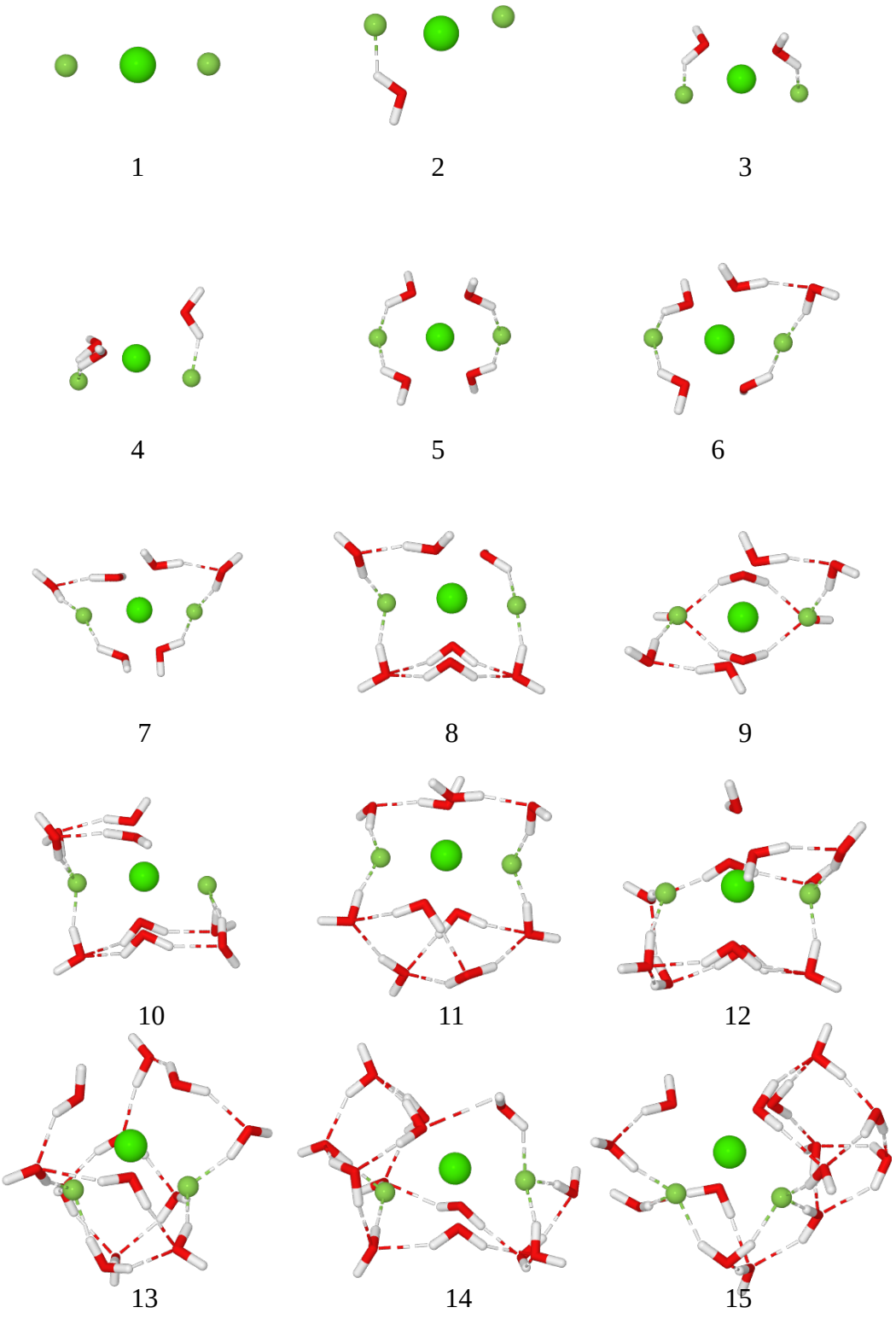

Fig. S3. Optimum structures for $CaF_2(H_2O)_n$, n = 1–14, calculated using MP2/6-311++G**.

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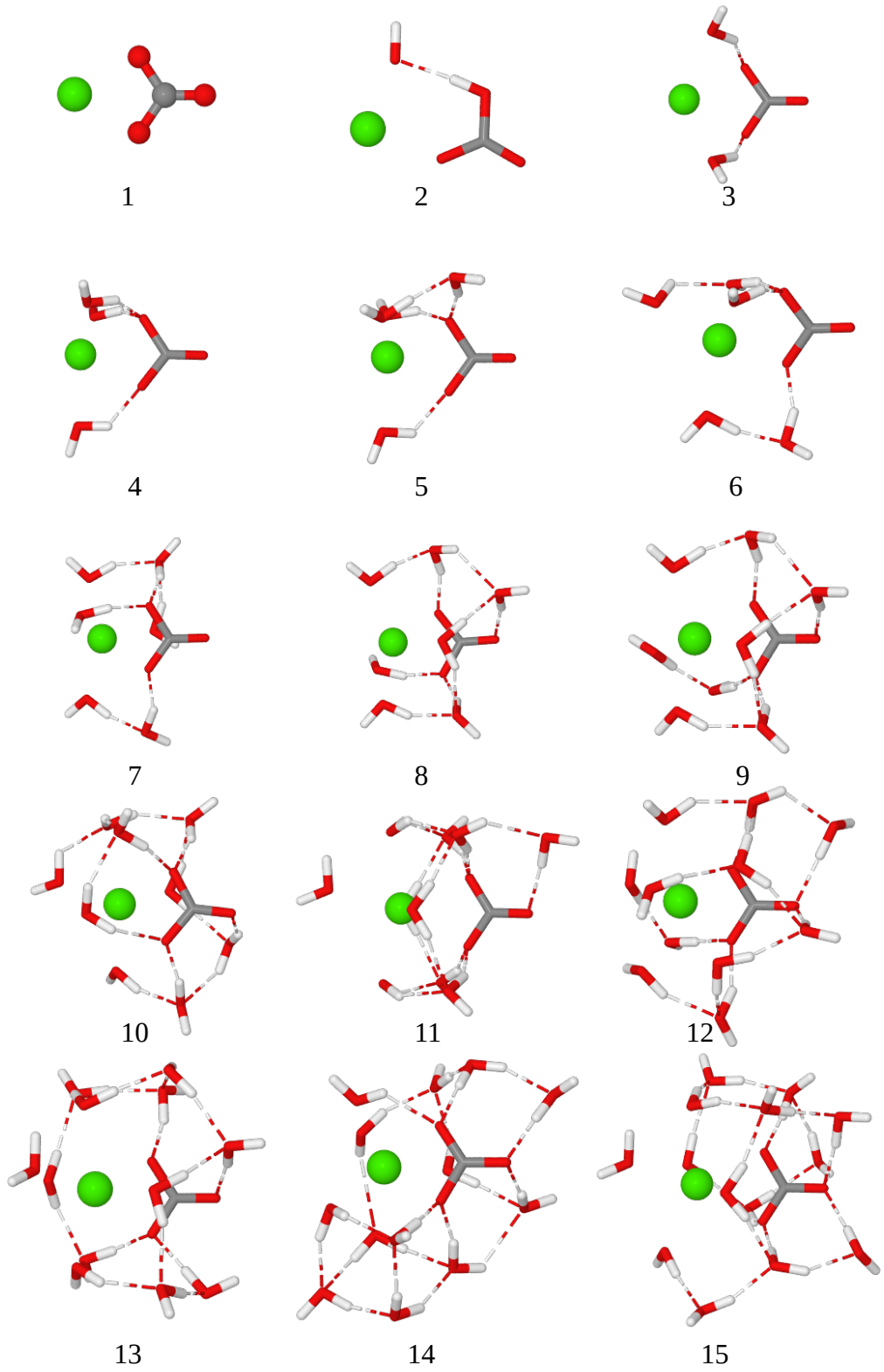

Fig. S4. Optimum structures for $CaCO_3(H_2O)_n$, n = 1–14, calculated using MP2/6-311++G**.

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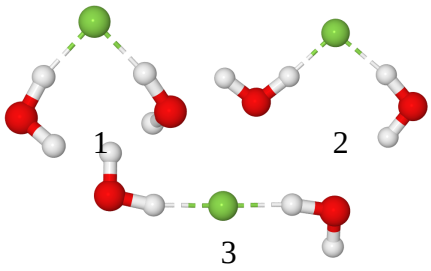

Fig. S5. $F^-(H_2O)_2$ minima at the HF/6-31G* level of theory.

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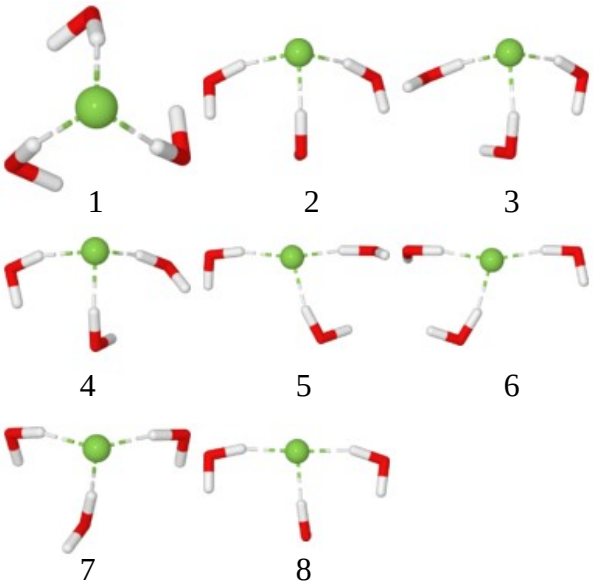

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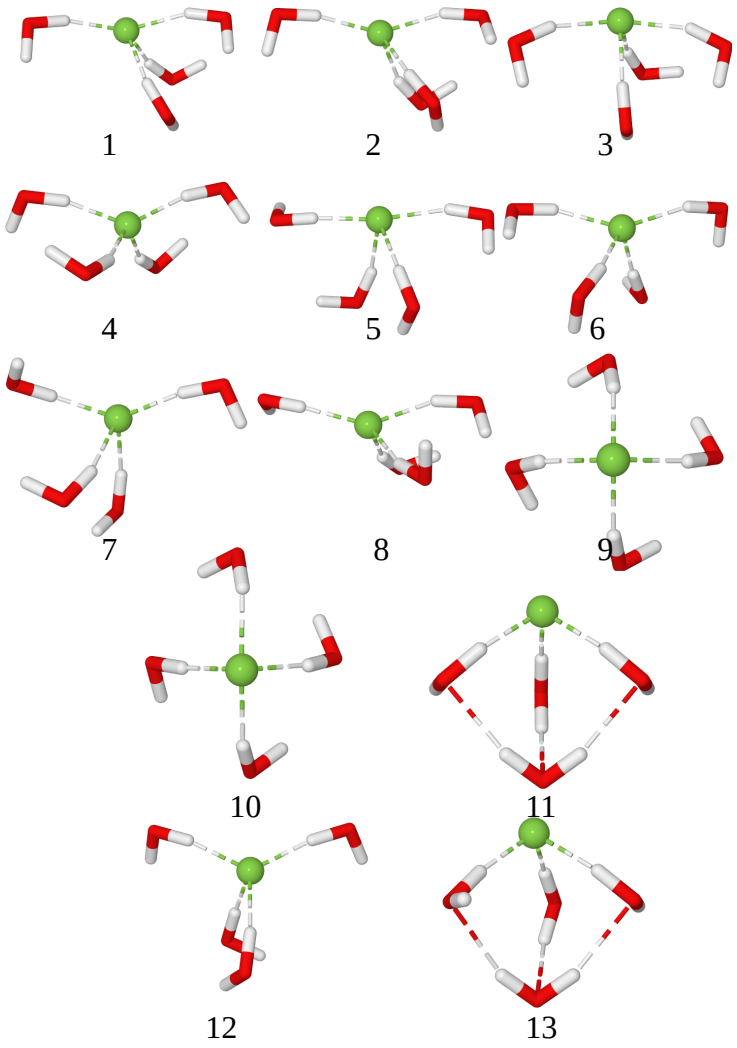

Fig. S7. $F^-(H_2O)_4$ minima at the HF/6-31G* level of theory.

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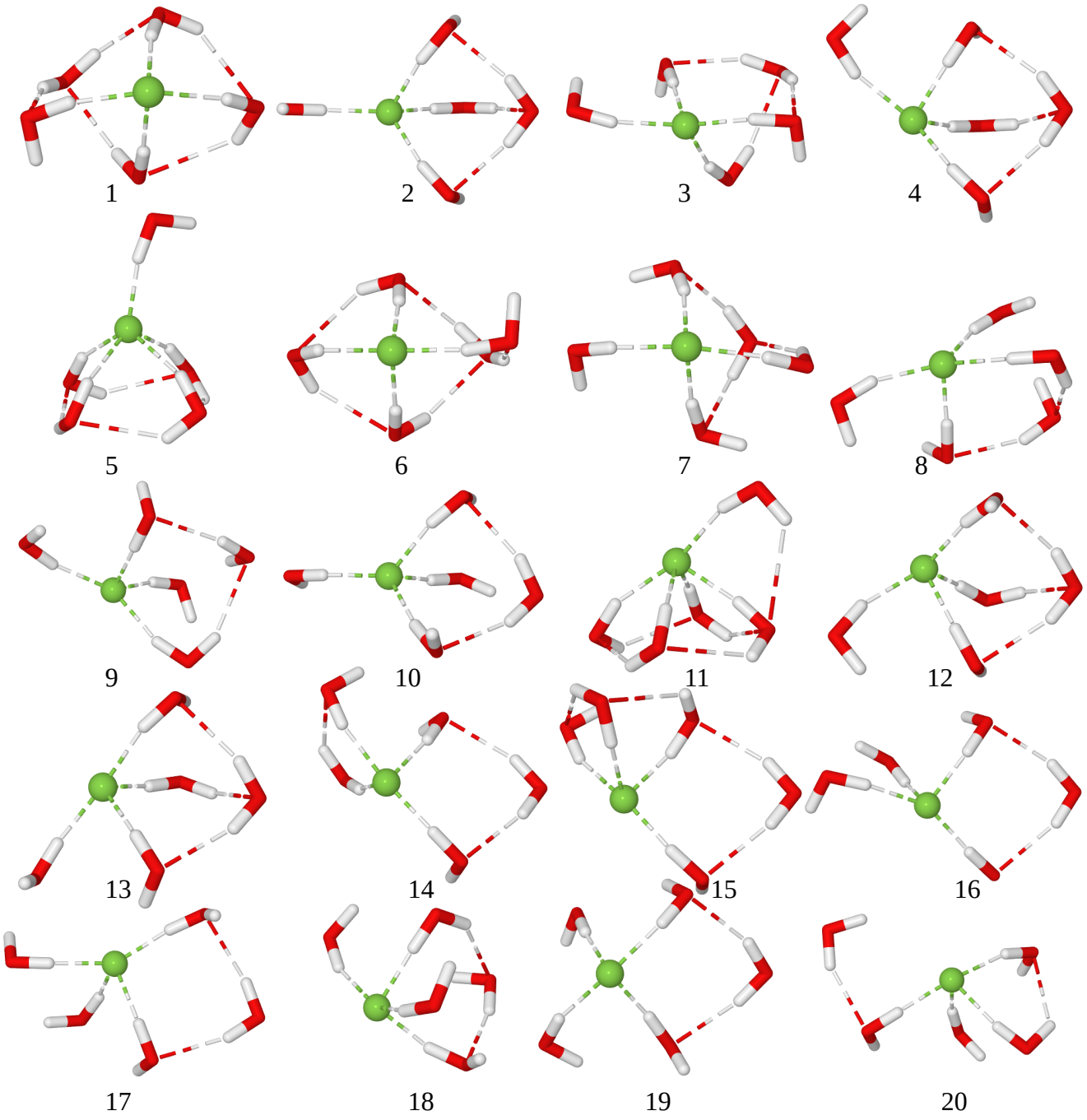

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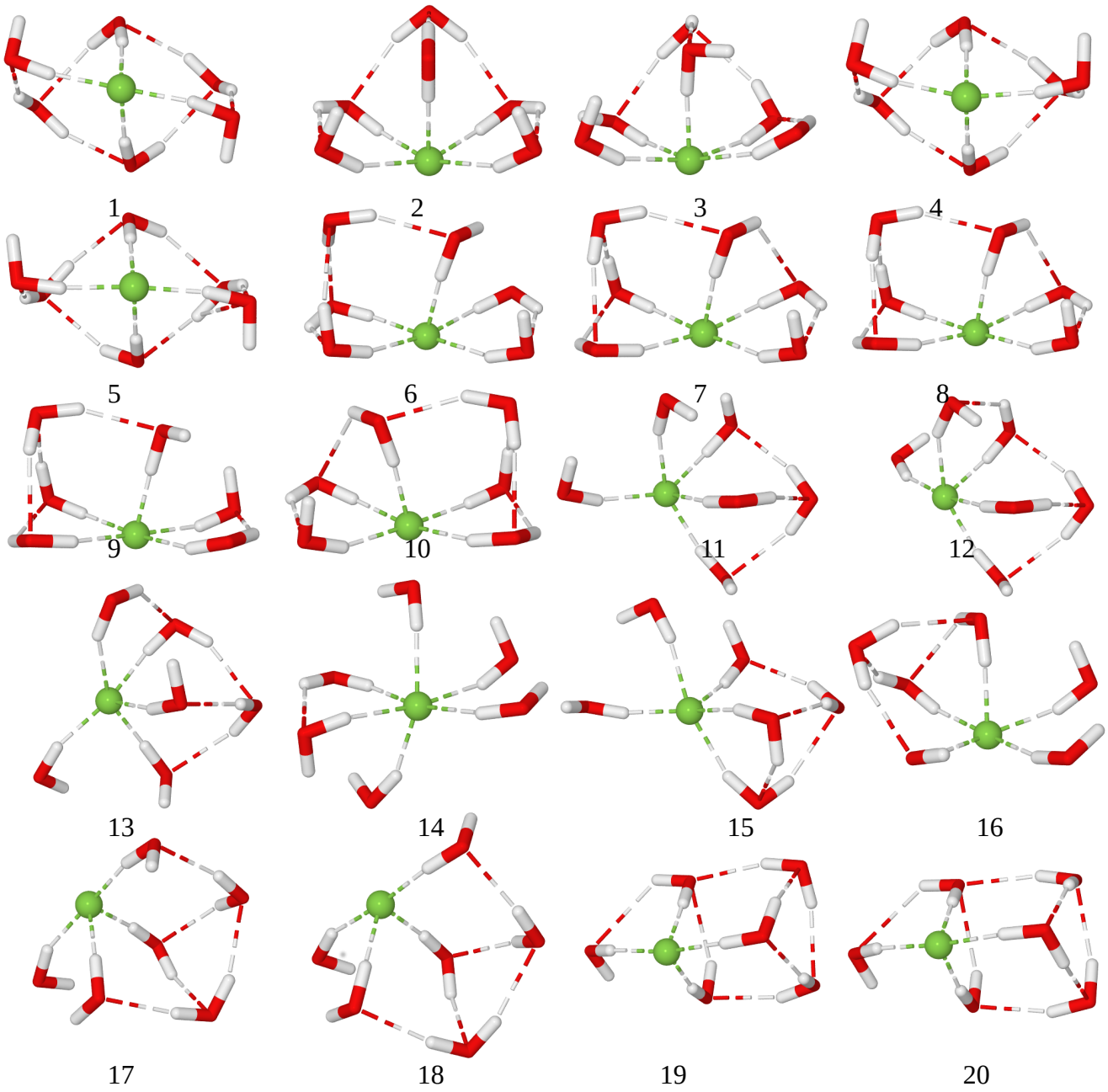

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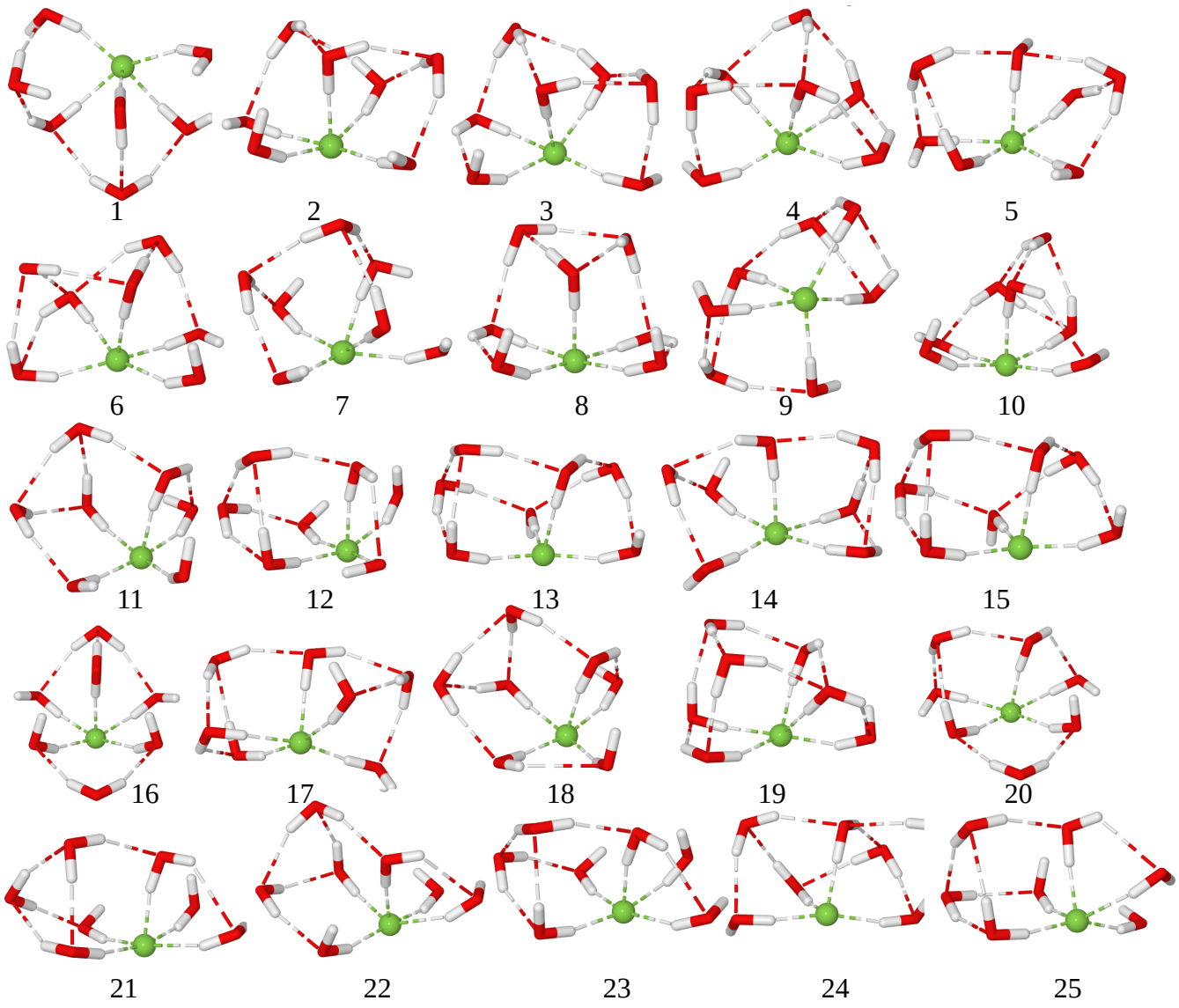

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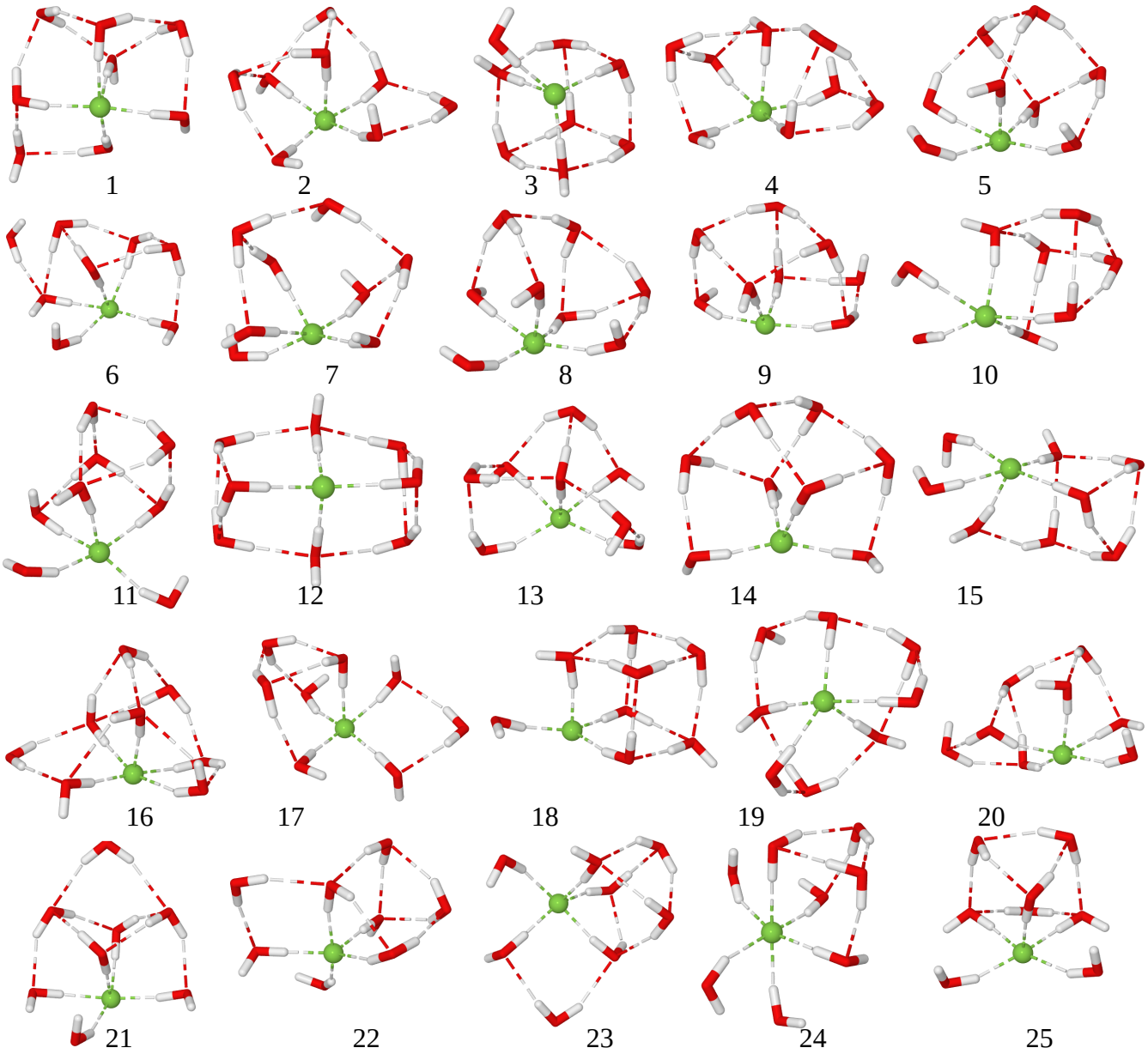

Fig. S11. $F^-(H_2O)_8$ minima at the HF/6-31G* level of theory.

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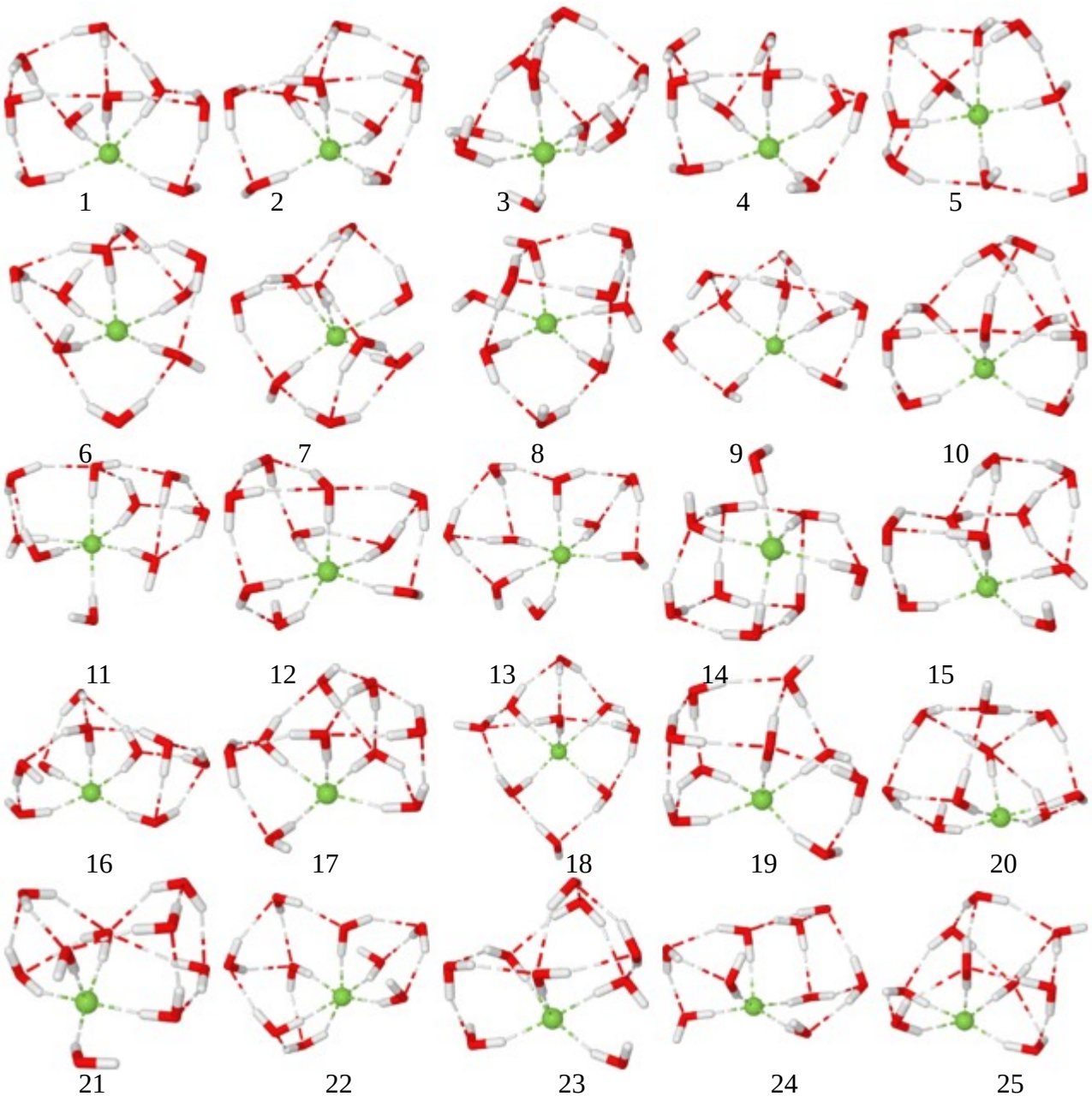

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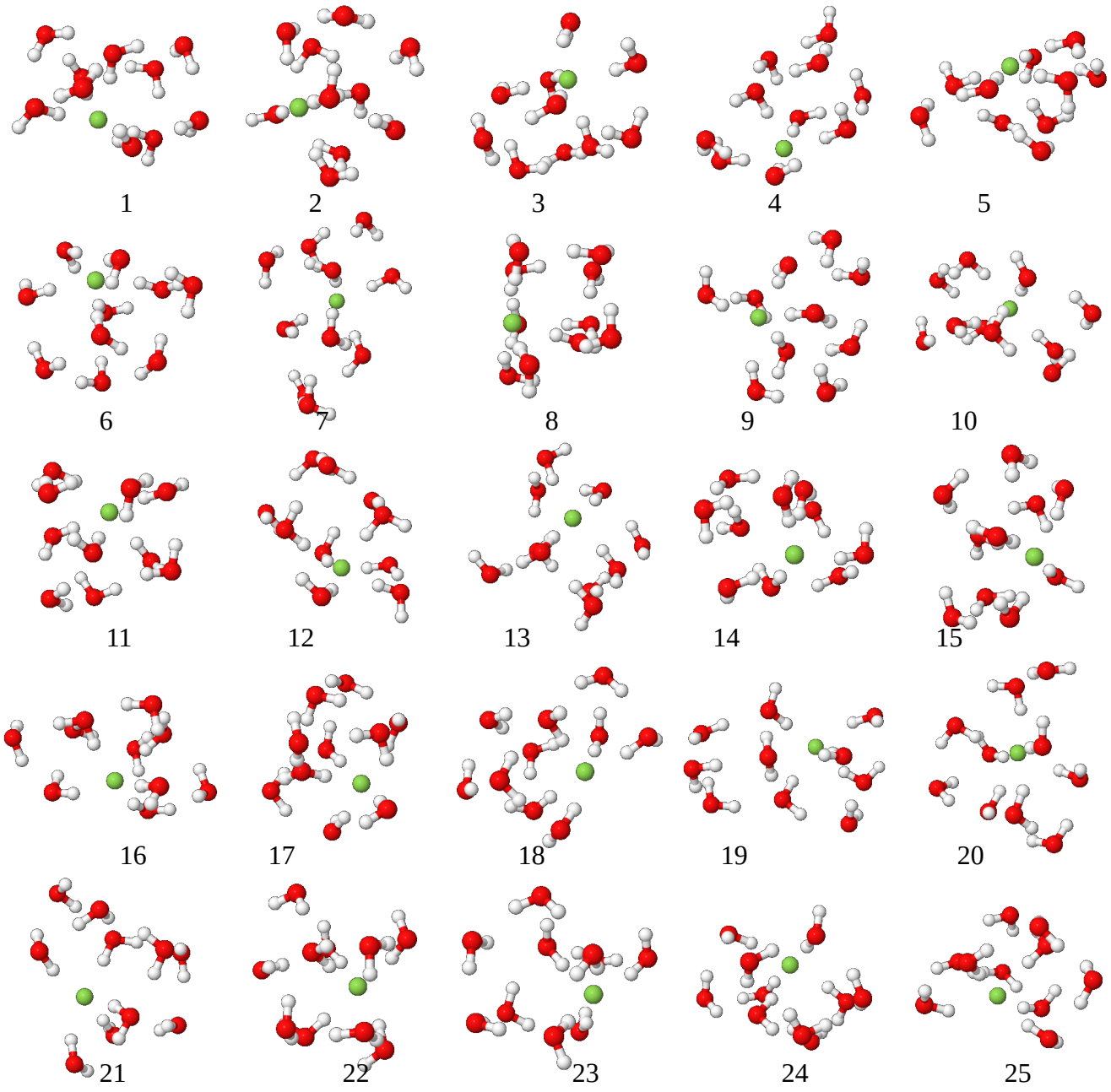

Fig. S13. $F^-(H_2O)_{10}$ minima at the HF/6-31G* level of theory.

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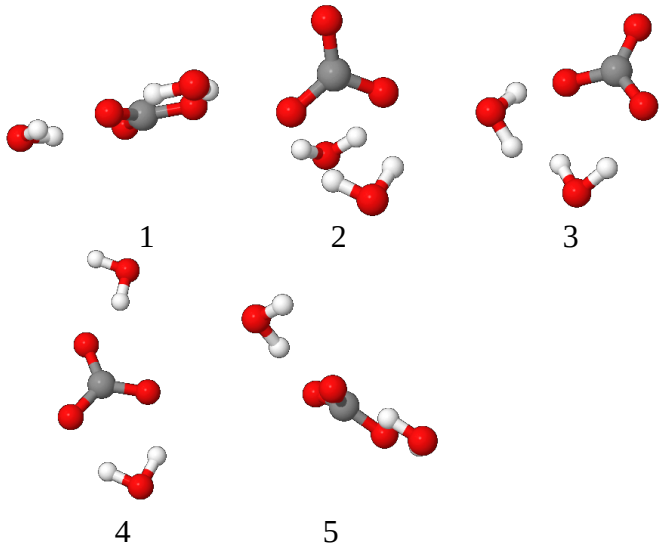

Fig. S14. $CO_3^{-2}(H_2O)_2$ minima at the HF/6-31G* level of theory.

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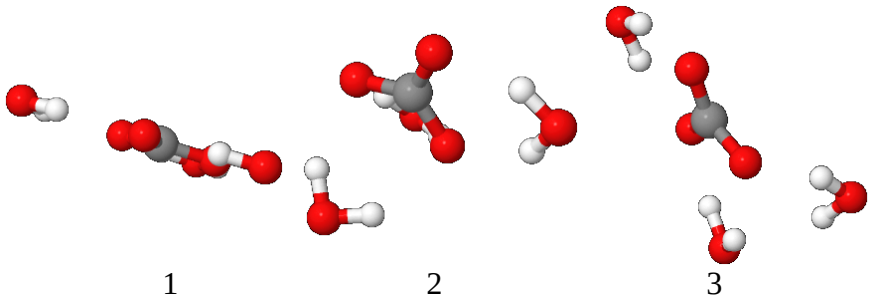

Fig. S15. $CO_3^{-2}(H_2O)_3$ minima at the HF/6-31G* level of theory.

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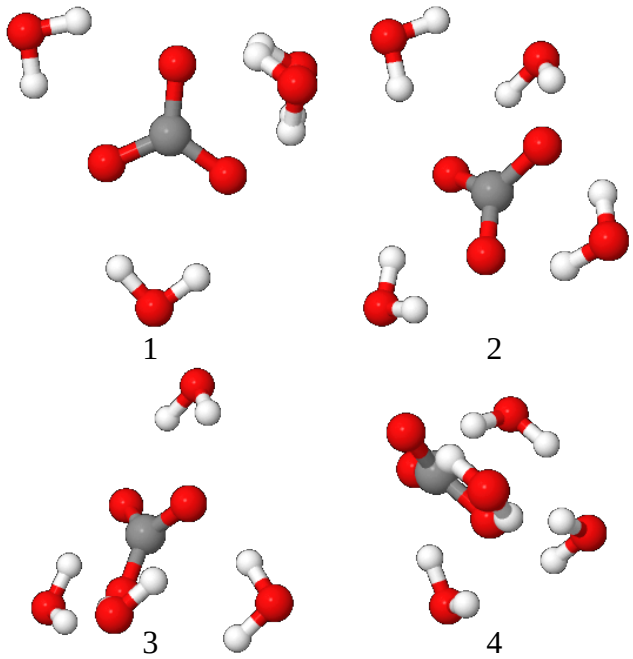

Fig. S16. $CO_3^{-2}(H_2O)_4$ minima at the HF/6-31G* level of theory.

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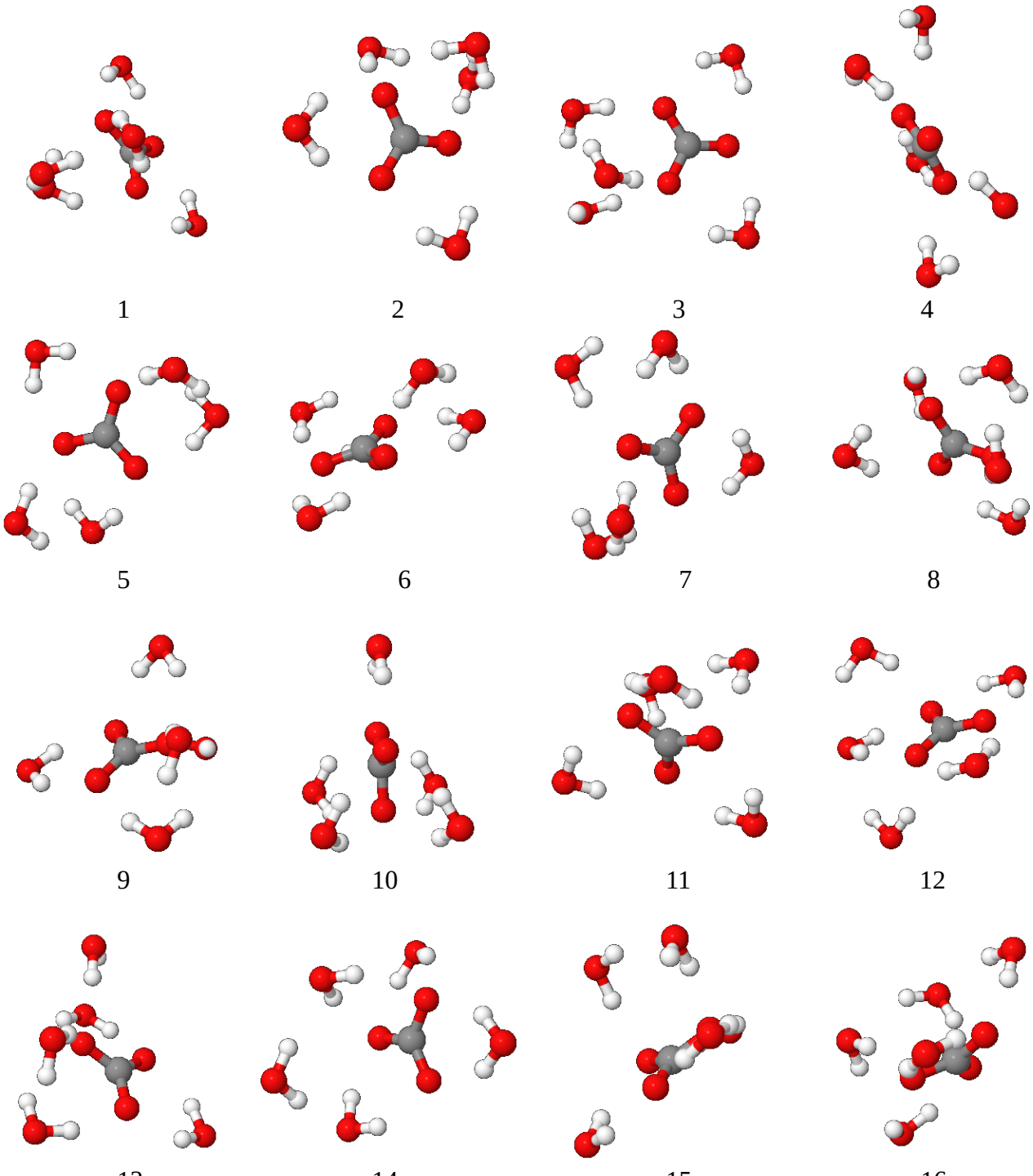

Fig. S17. $CO_3^{-2}(H_2O)_5$ minima at the HF/6-31G* level of theory.

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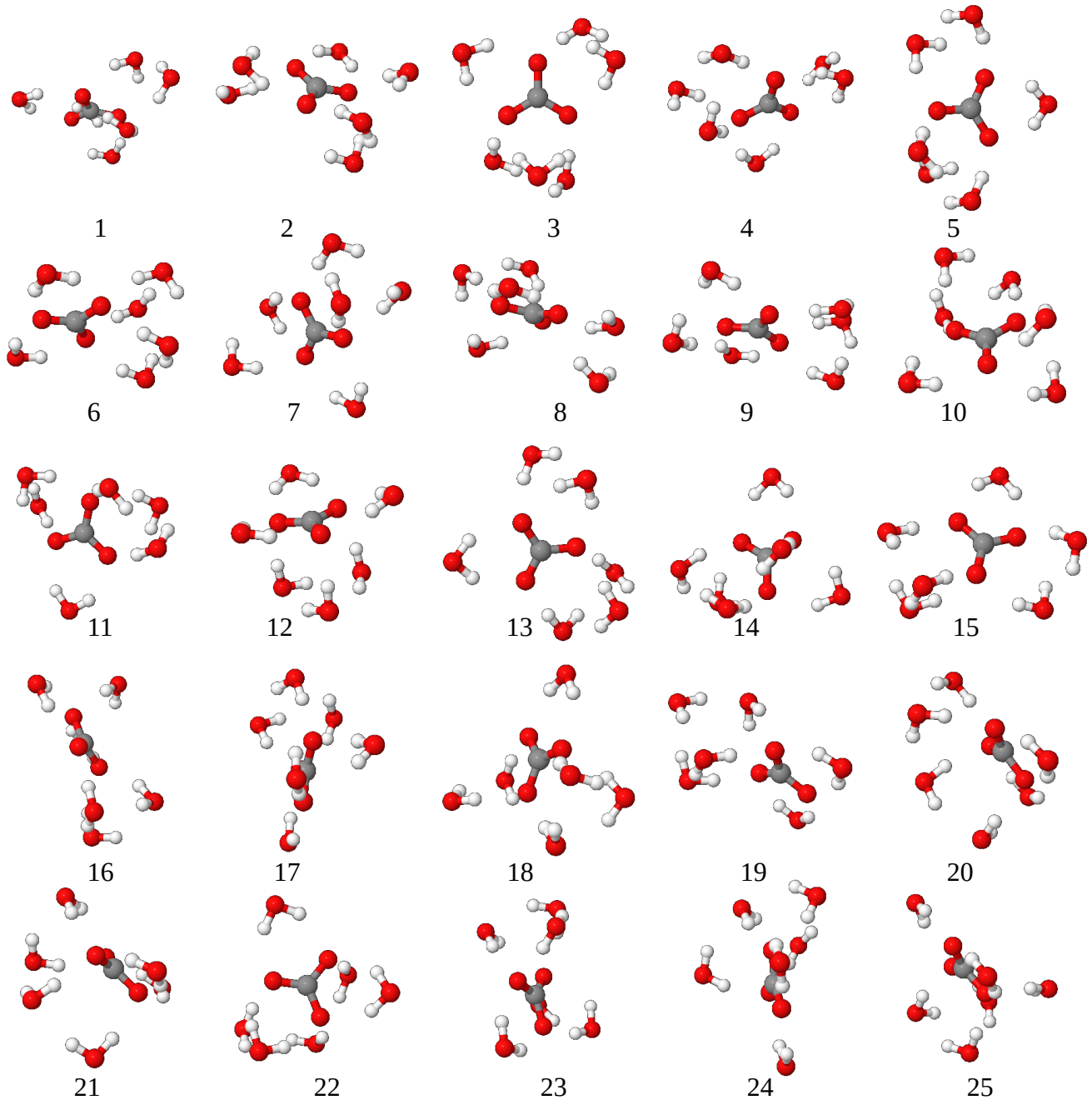

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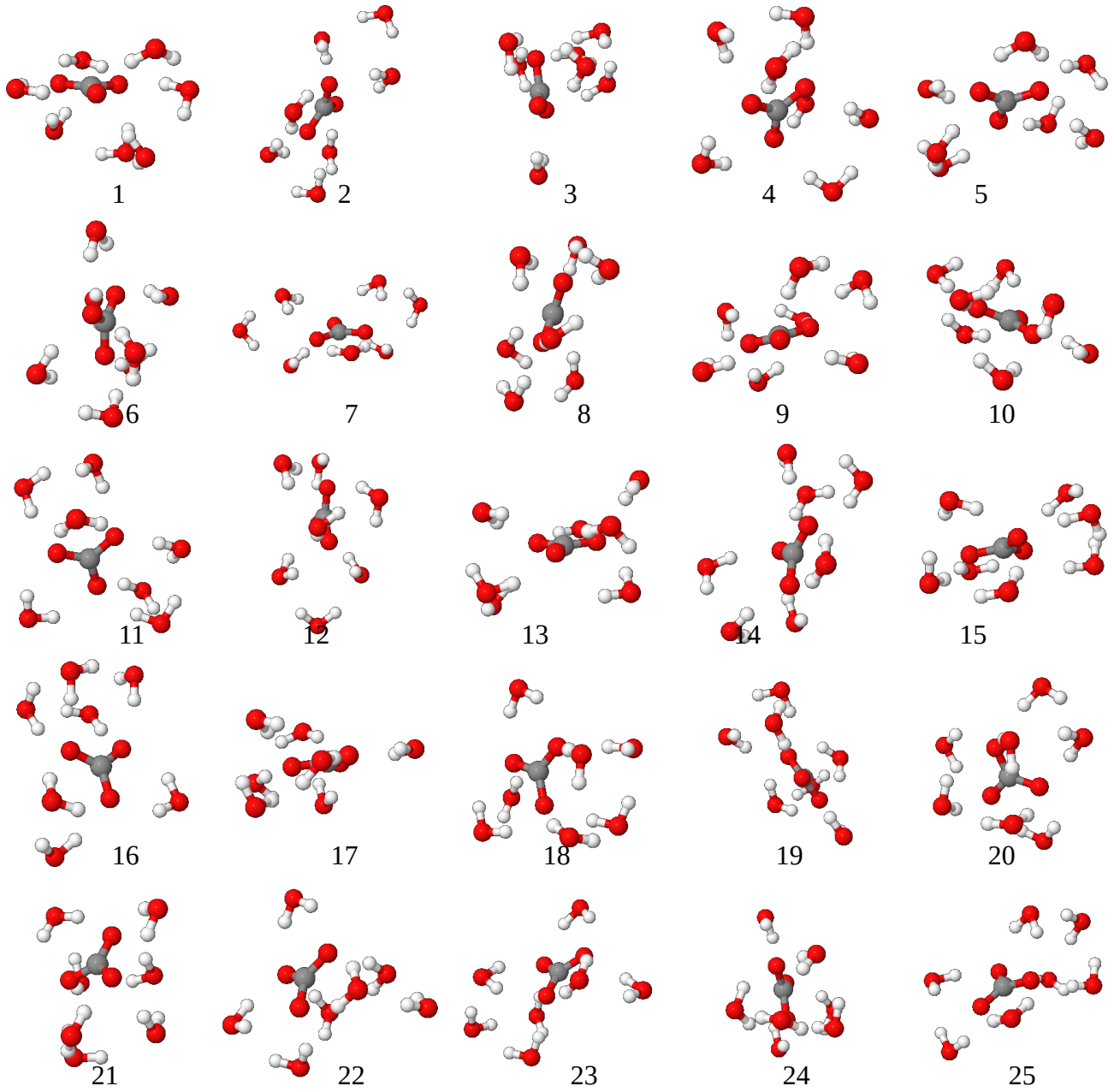

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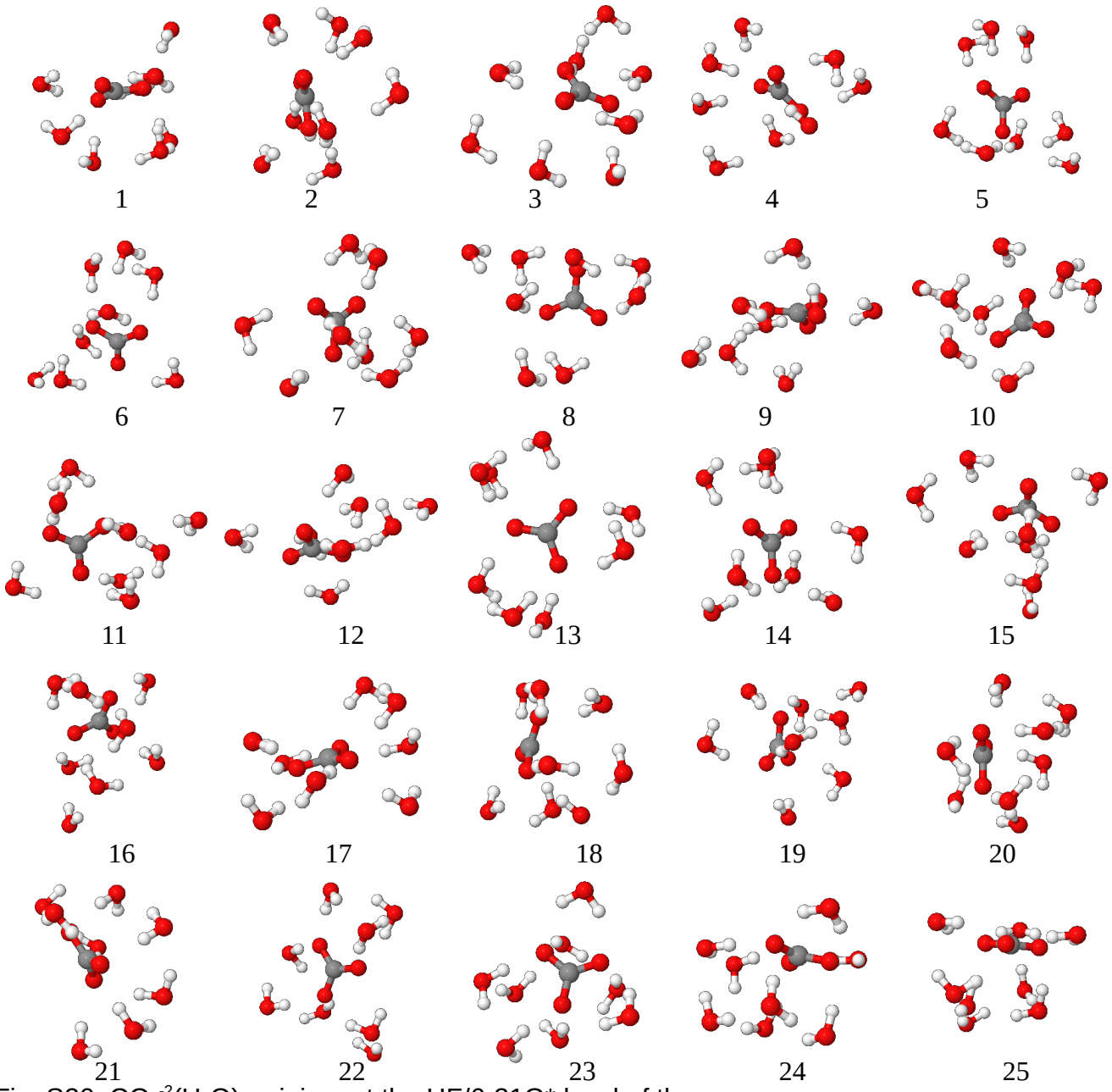

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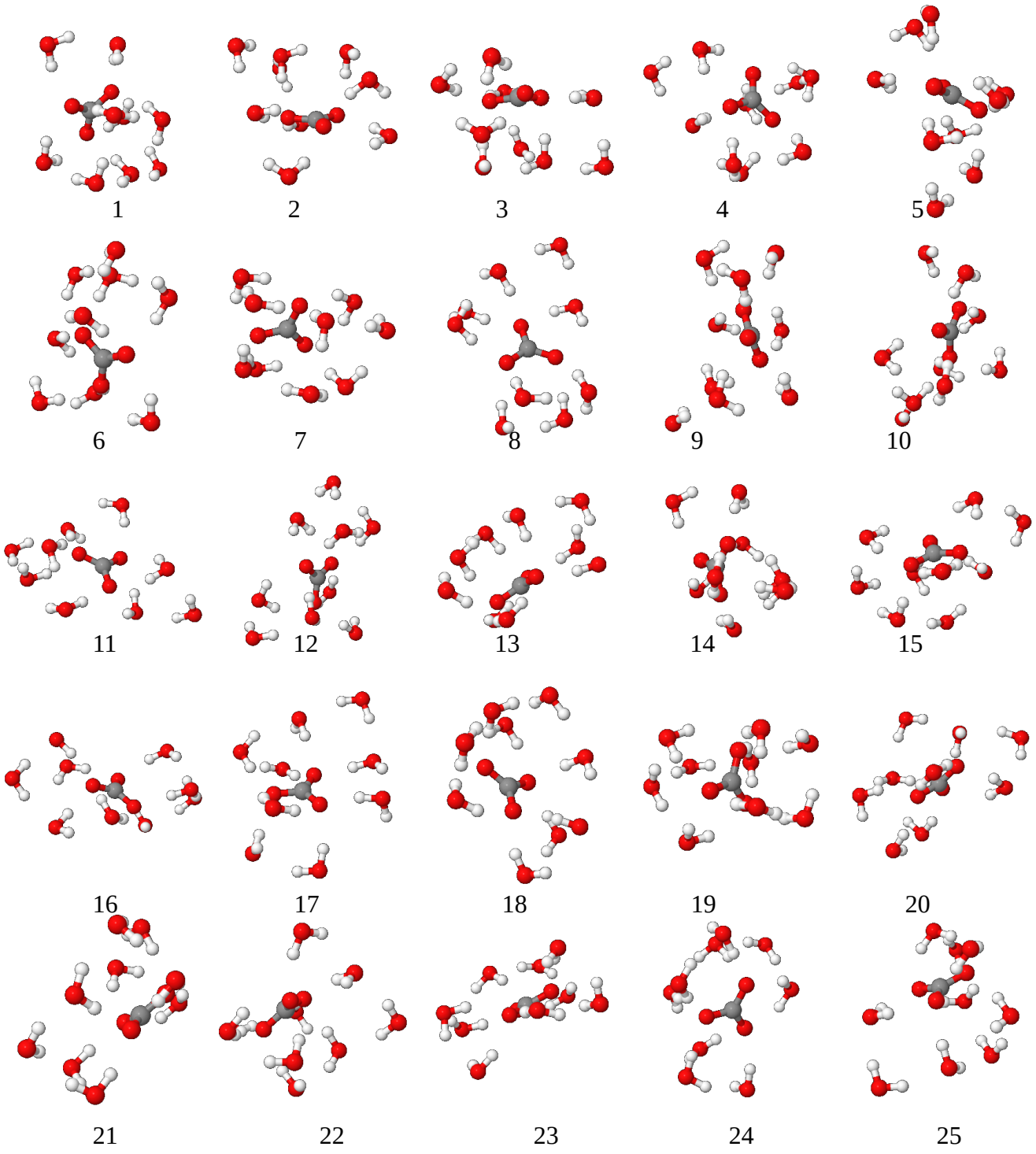

Fig. S21. $CO_3^{-2}(H_2O)_9$ minima at the HF/6-31G* level of theory.

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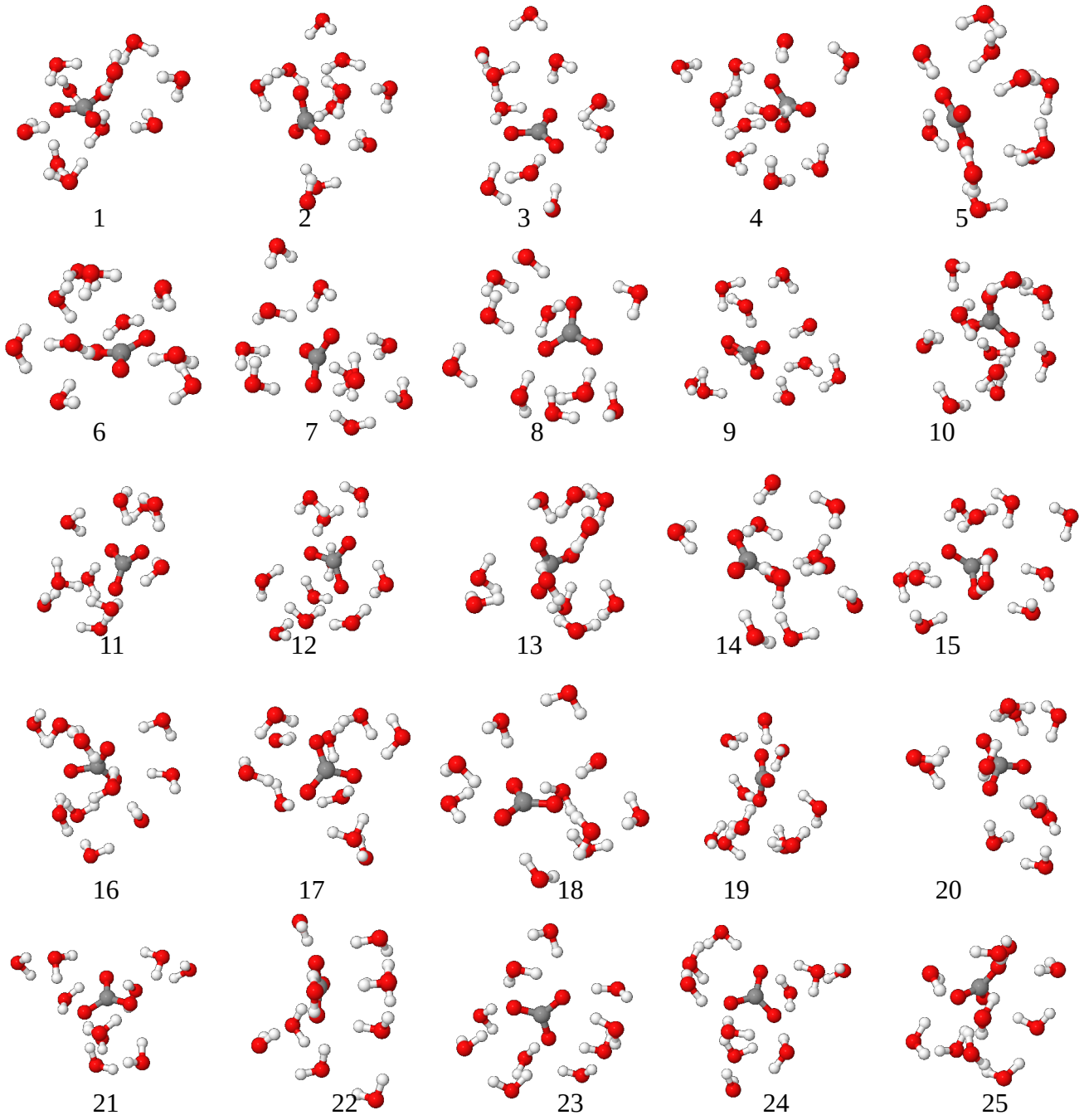

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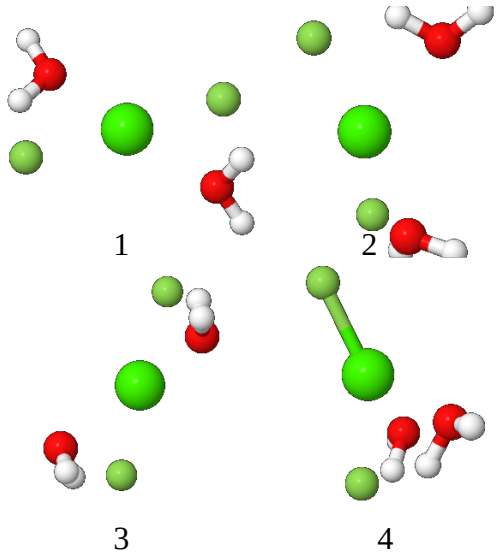

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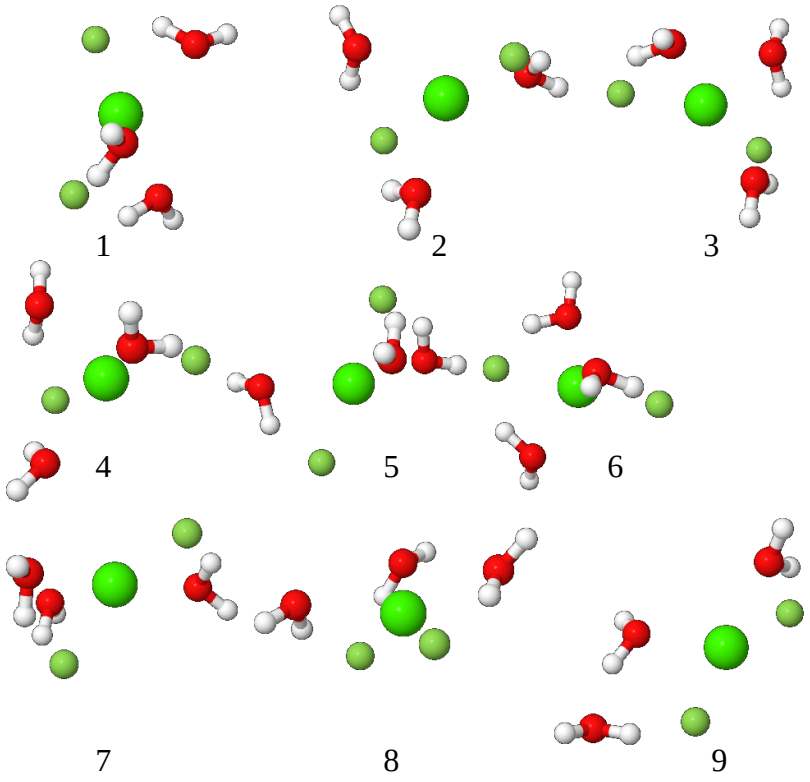

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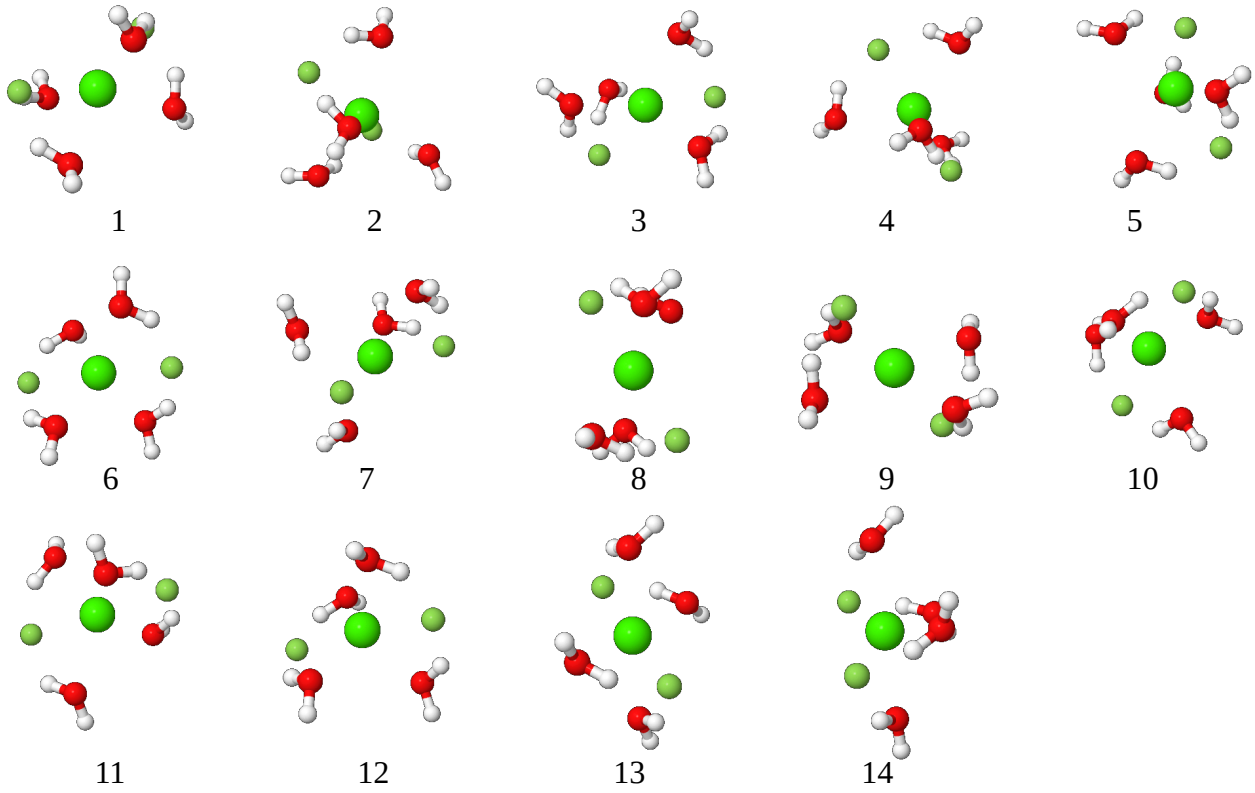

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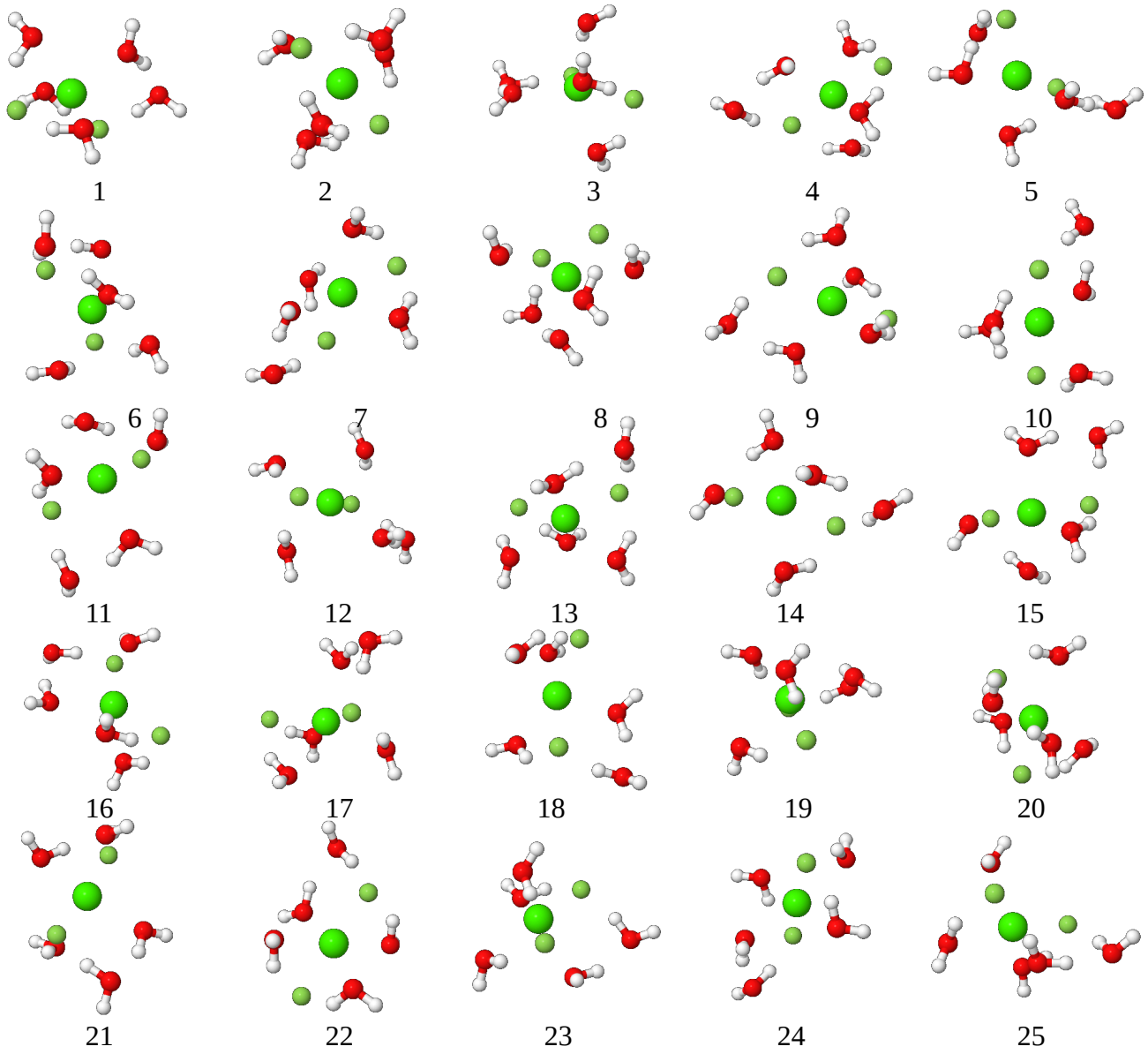

Fig. S26. $CaF_2(H_2O)_5$ minima at the HF/6-31G* level of theory.

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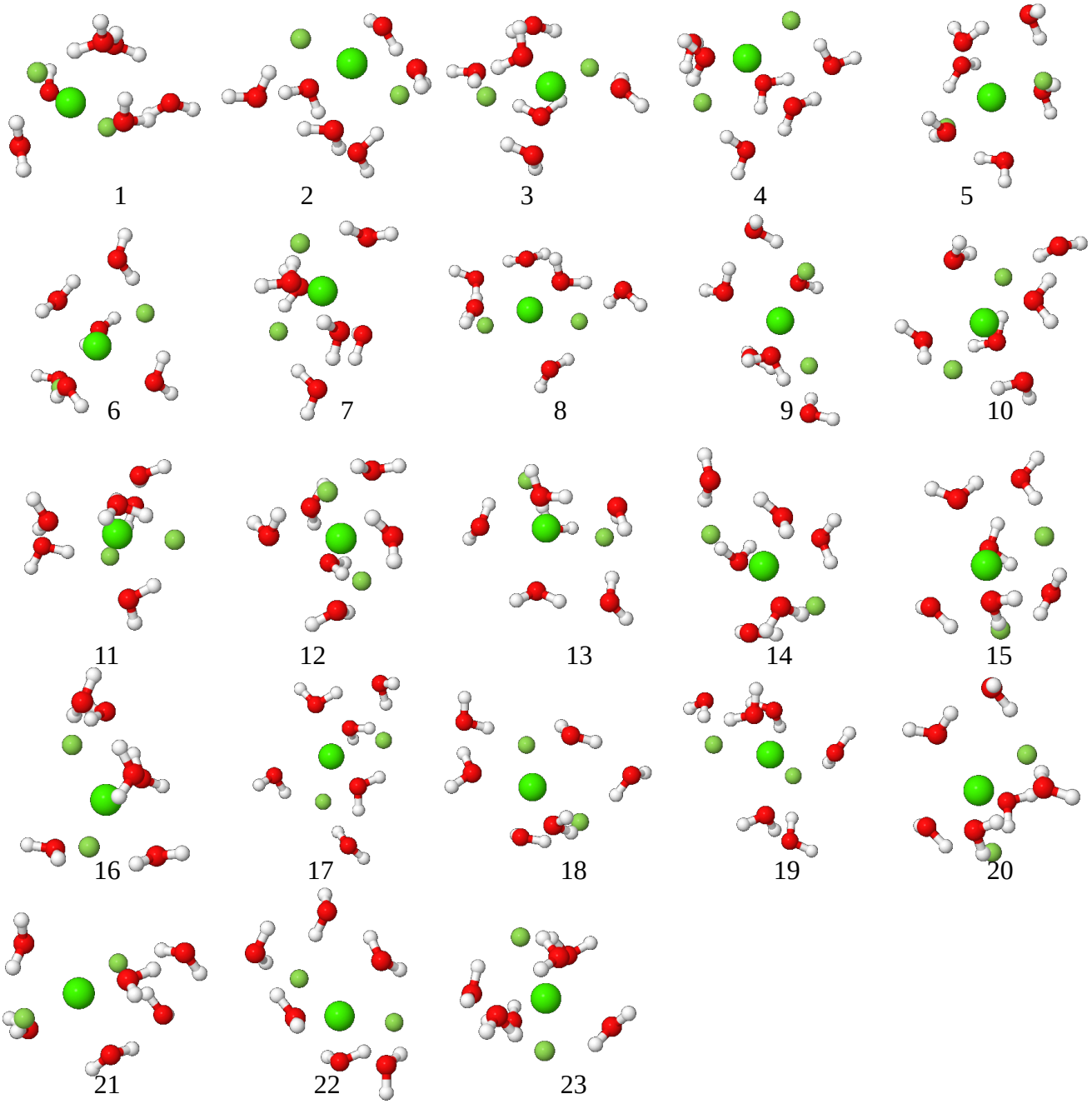

Fig. S27. $CaF_2(H_2O)_6$ minima at the HF/6-31G* level of theory.

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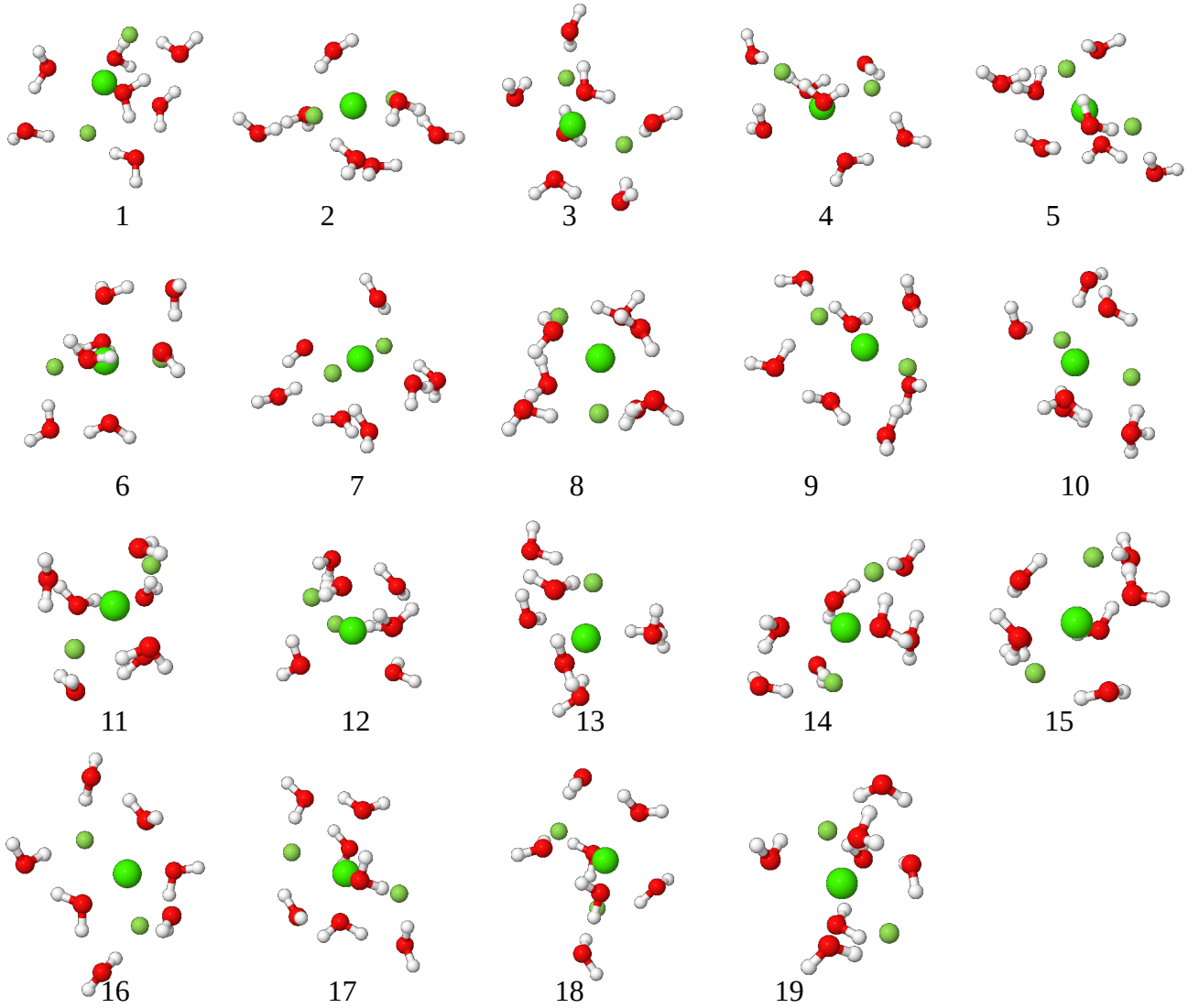

Fig. S28. $CaF_2(H_2O)_7$ minima at the HF/6-31G* level of theory.

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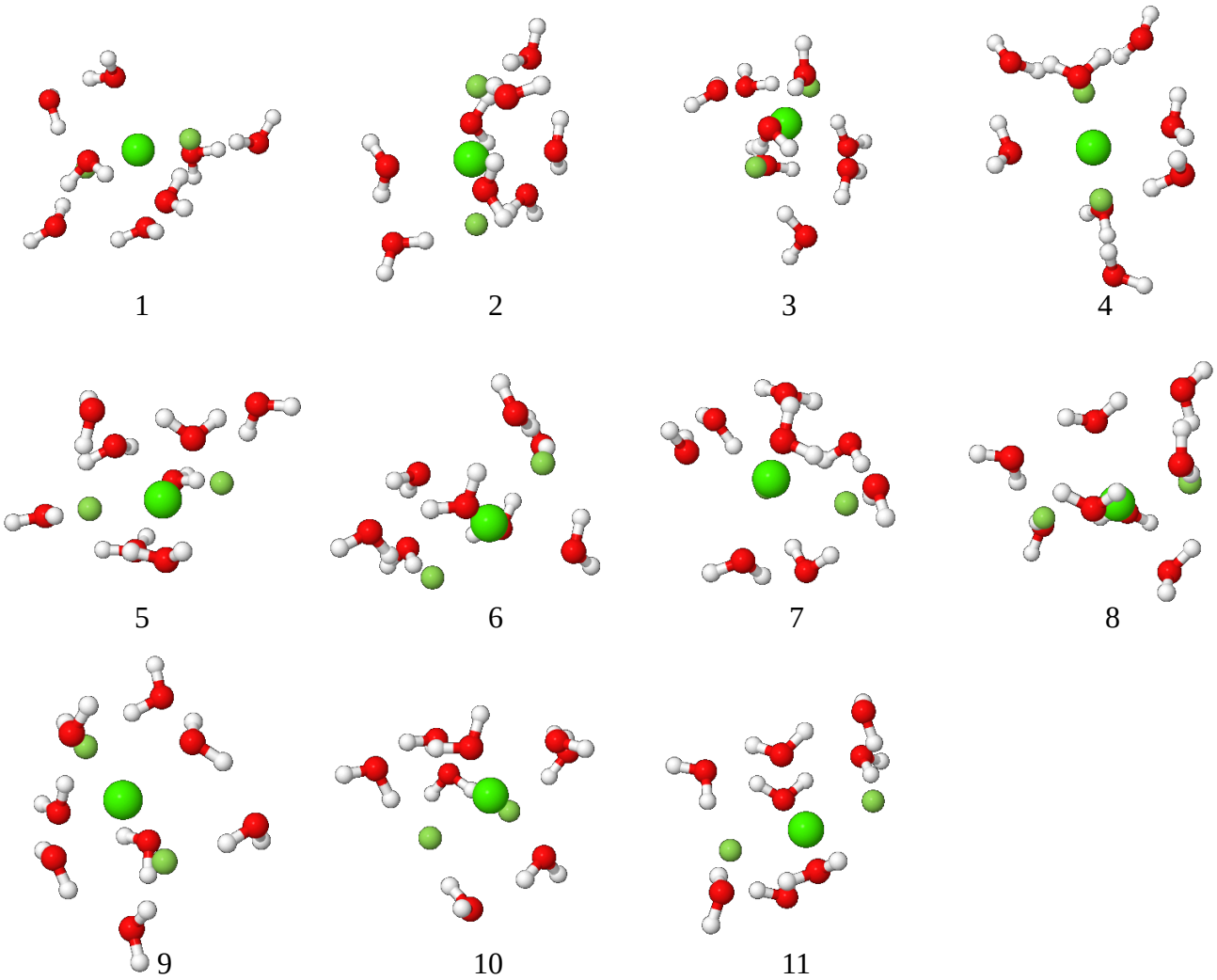

Fig. S29. $CaF_2(H_2O)_8$ minima at the HF/6-31G* level of theory.

Structures in XYZ format available at DOI: 10.6084/m9.figshare.7073243
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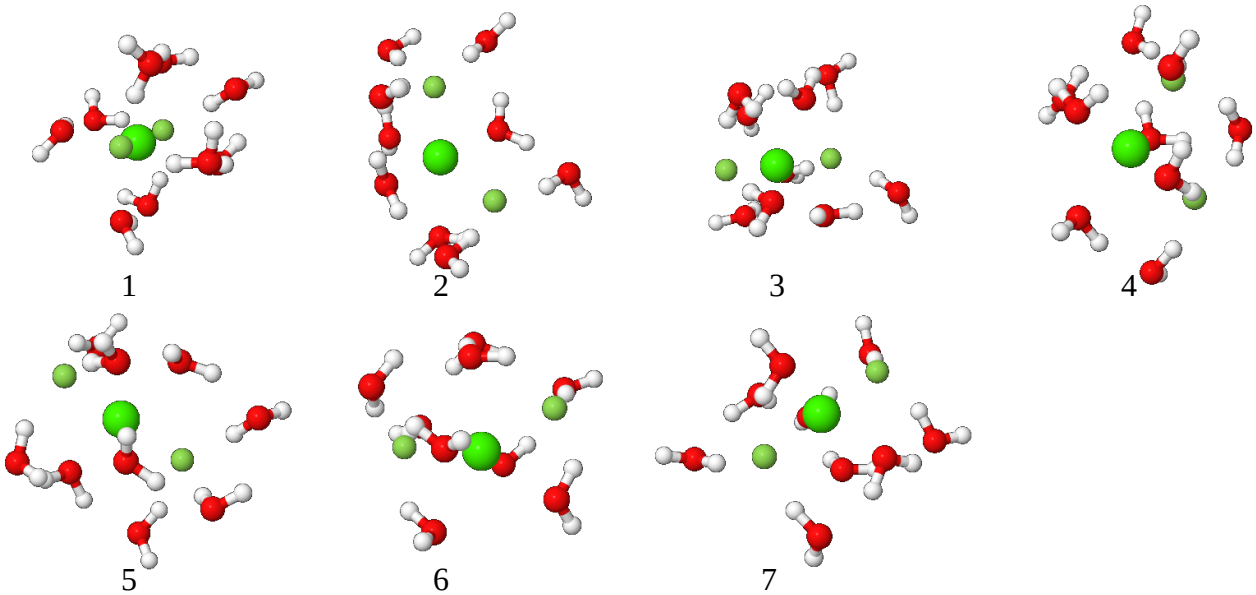

Fig. S30. $CaF_2(H_2O)_9$ minima at the HF/6-31G* level of theory.

Structures in XYZ format available at DOI: 10.6084/m9.figshare.7073252
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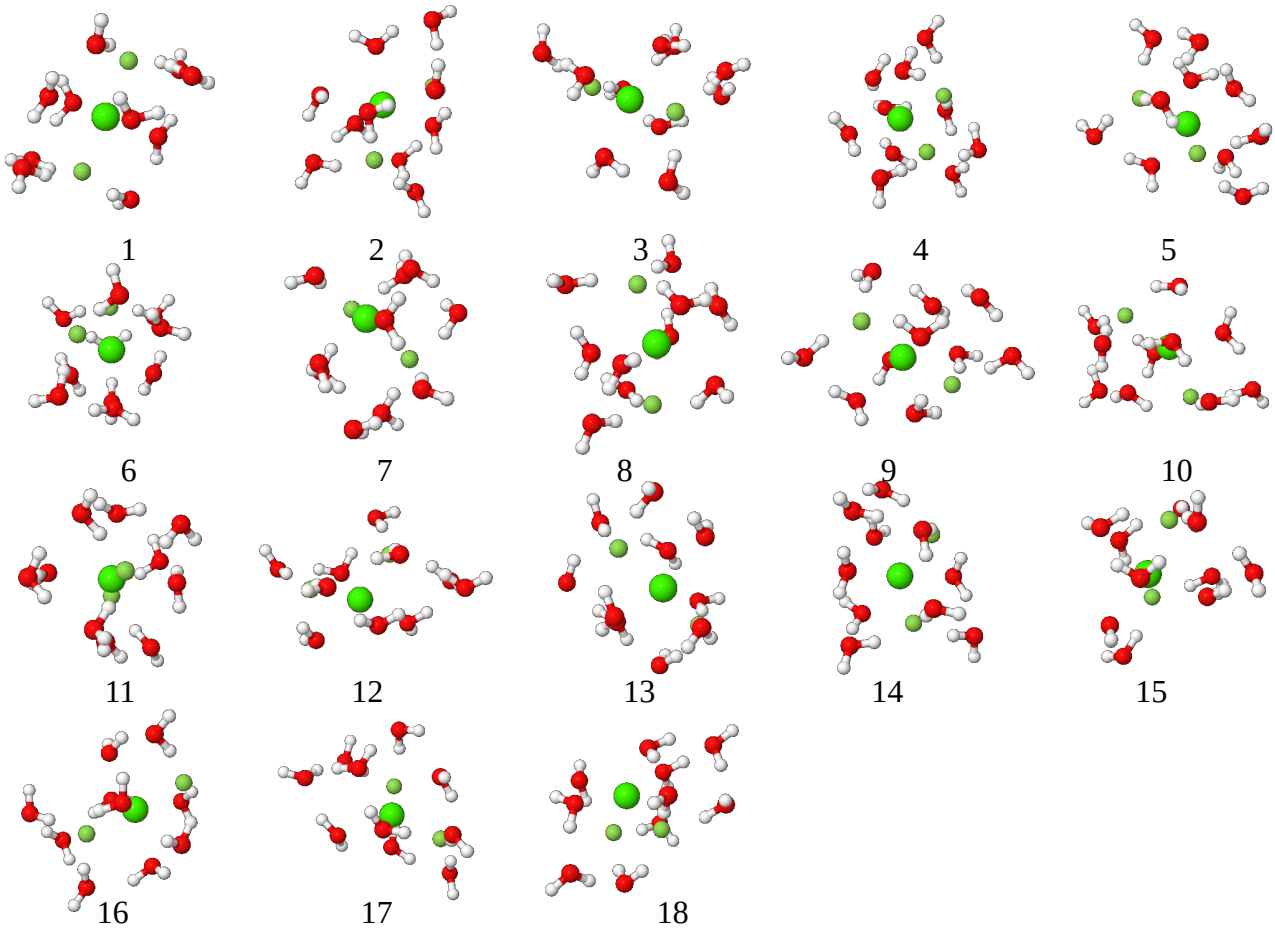

Fig. S31. $CaF_2(H_2O)_{10}$ minima at the HF/6-31G* level of theory.

Structures in XYZ format available at DOI: 10.6084/m9.figshare.7073258
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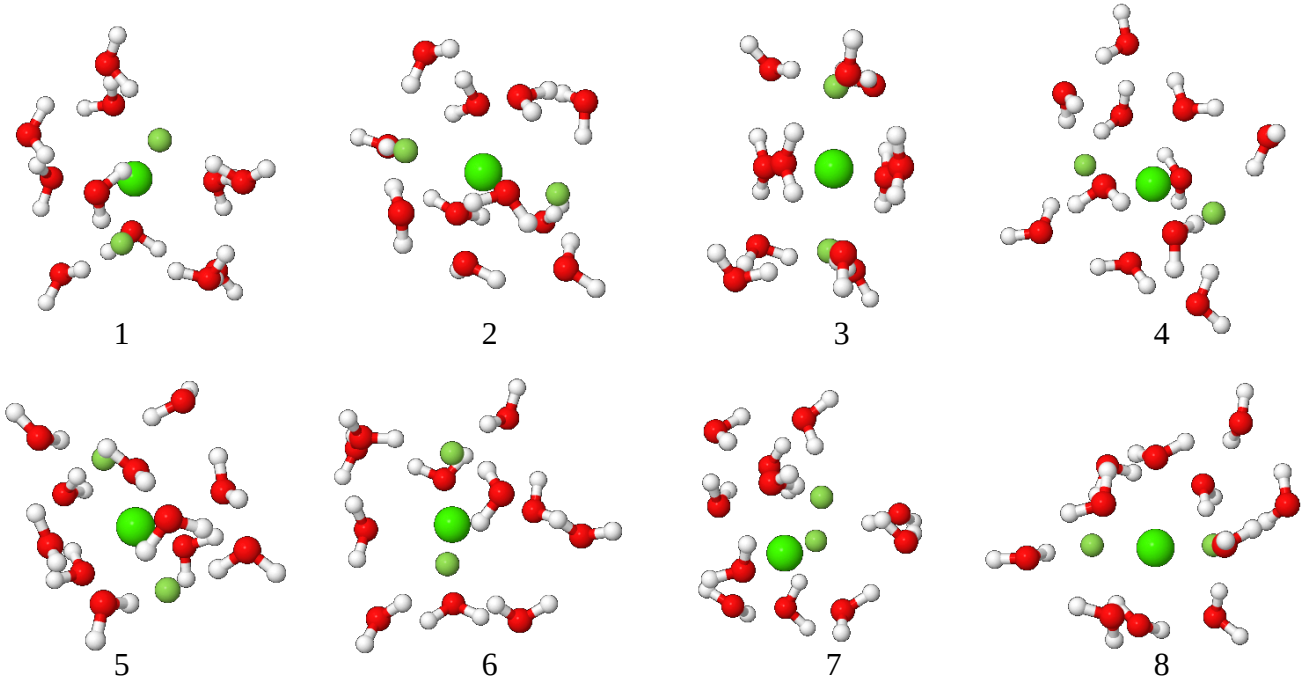

Fig. S32. $CaF_2(H_2O)_{11}$ minima at the HF/6-31G* level of theory.

Structures in XYZ format available at DOI: 10.6084/m9.figshare.7073270
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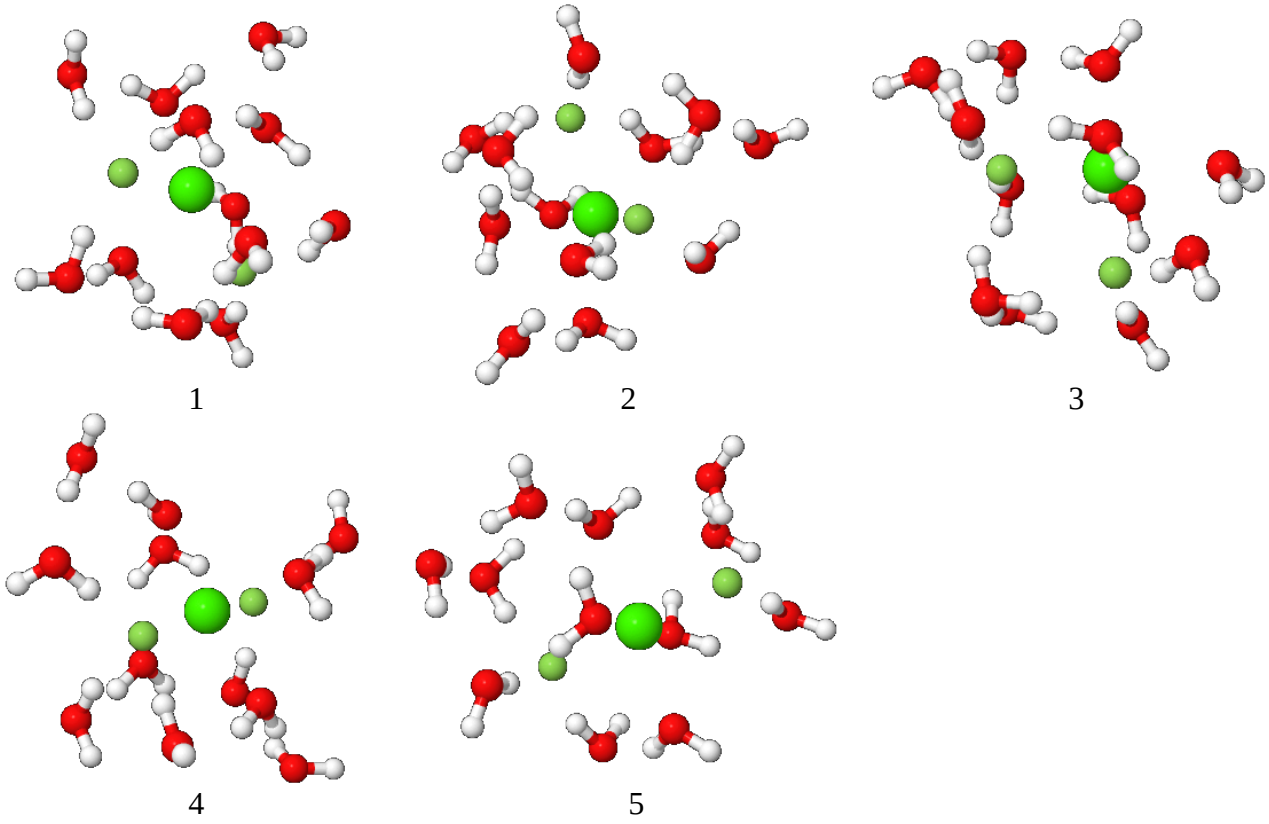

Fig. S33. $CaF_2(H_2O)_{12}$ minima at the HF/6-31G* level of theory.

Structures in XYZ format available at DOI: 10.6084/m9.figshare.7073273
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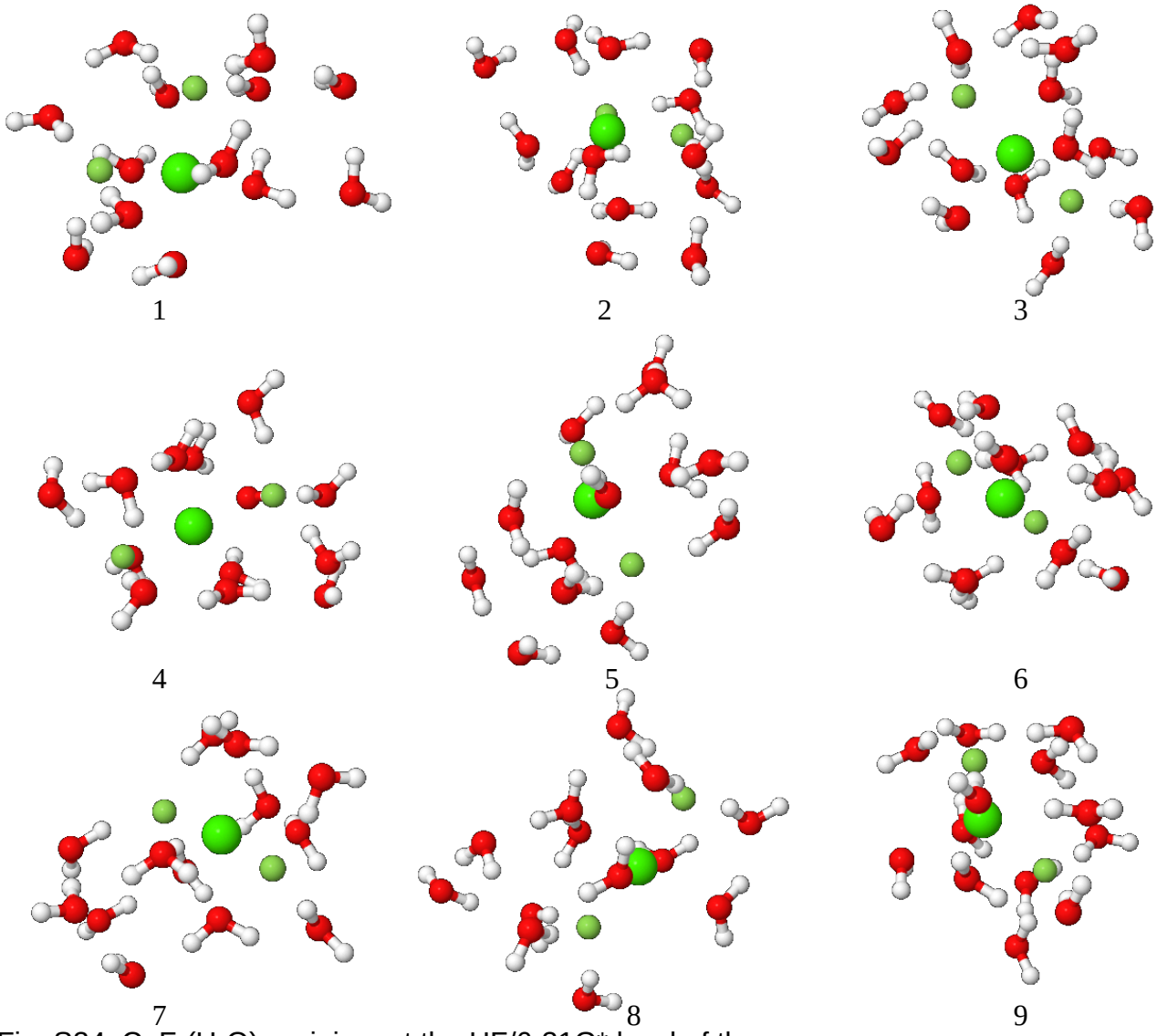

Fig. S34. $CaF_2(H_2O)_{13}$ minima at the HF/6-31G* level of theory.

Structures in XYZ format available at DOI: 10.6084/m9.figshare.7073276
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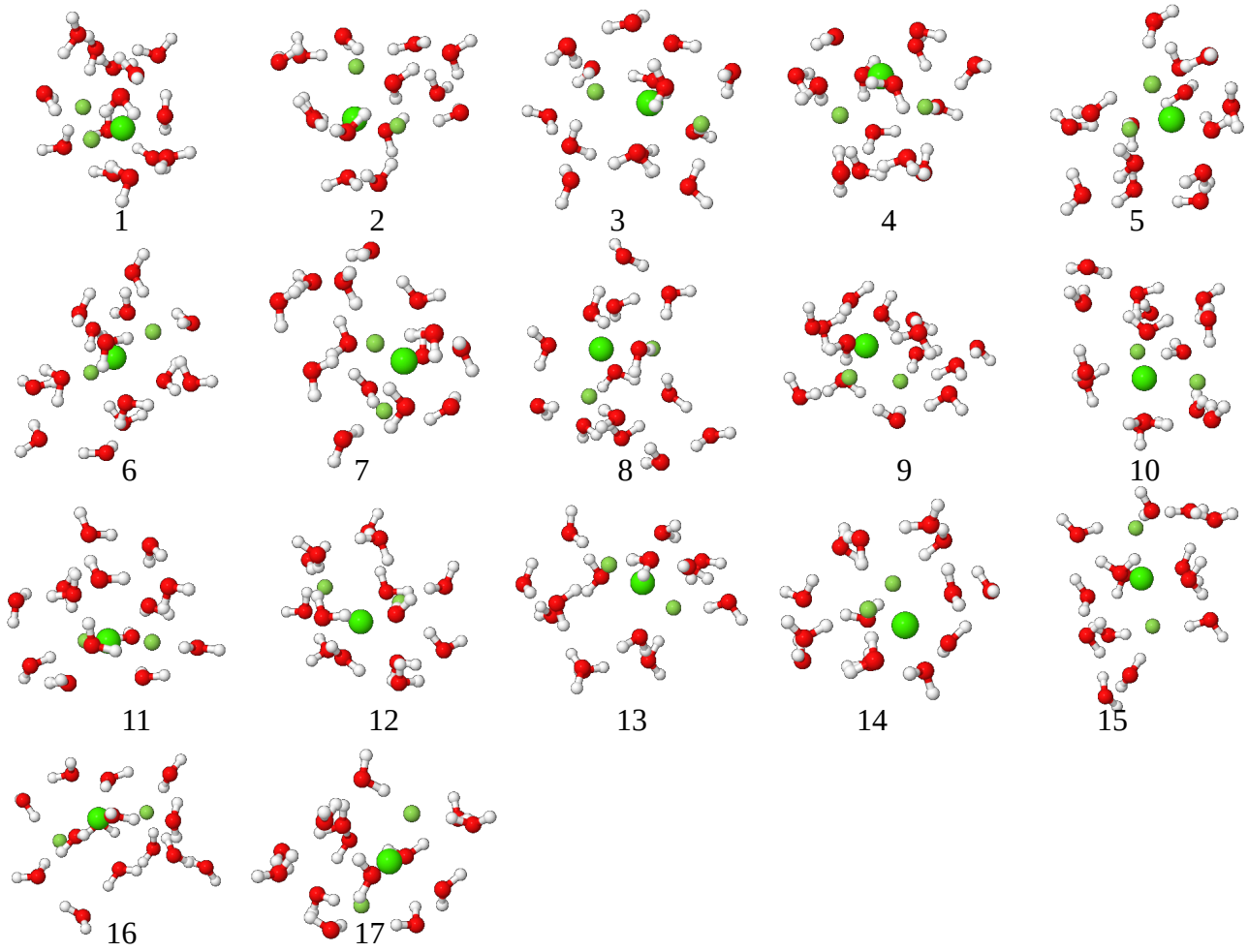

Fig. S35. $CaF_2(H_2O)_{14}$ minima at the HF/6-31G* level of theory.

Structures in XYZ format available at DOI: 10.6084/m9.figshare.7073282
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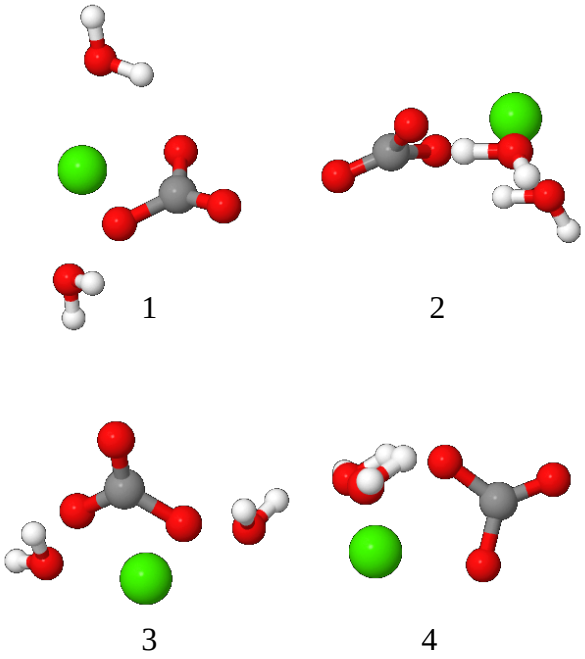

Fig. S36. $CaCO_3(H_2O)_2$ minima at the HF/6-31G* level of theory.

Structures in XYZ format available at DOI: 10.6084/m9.figshare.7077200
https://figshare.com/s/cc4c6f112892302b0115

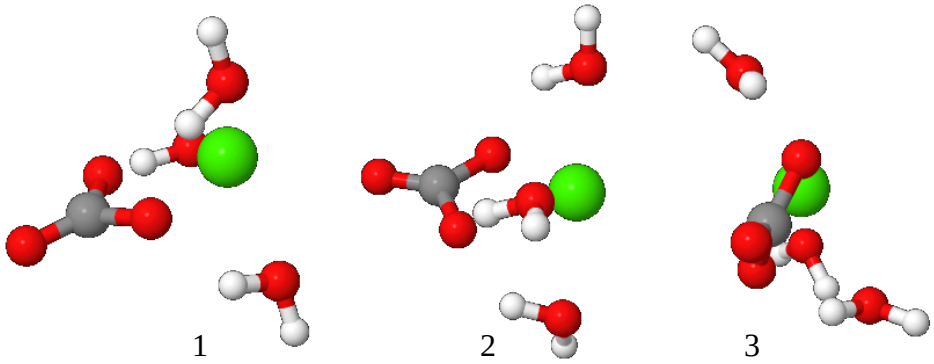

Fig. S37. $CaCO_3(H_2O)_3$ minima at the HF/6-31G* level of theory.

Structures in XYZ format available at DOI: 10.6084/m9.figshare.7077206
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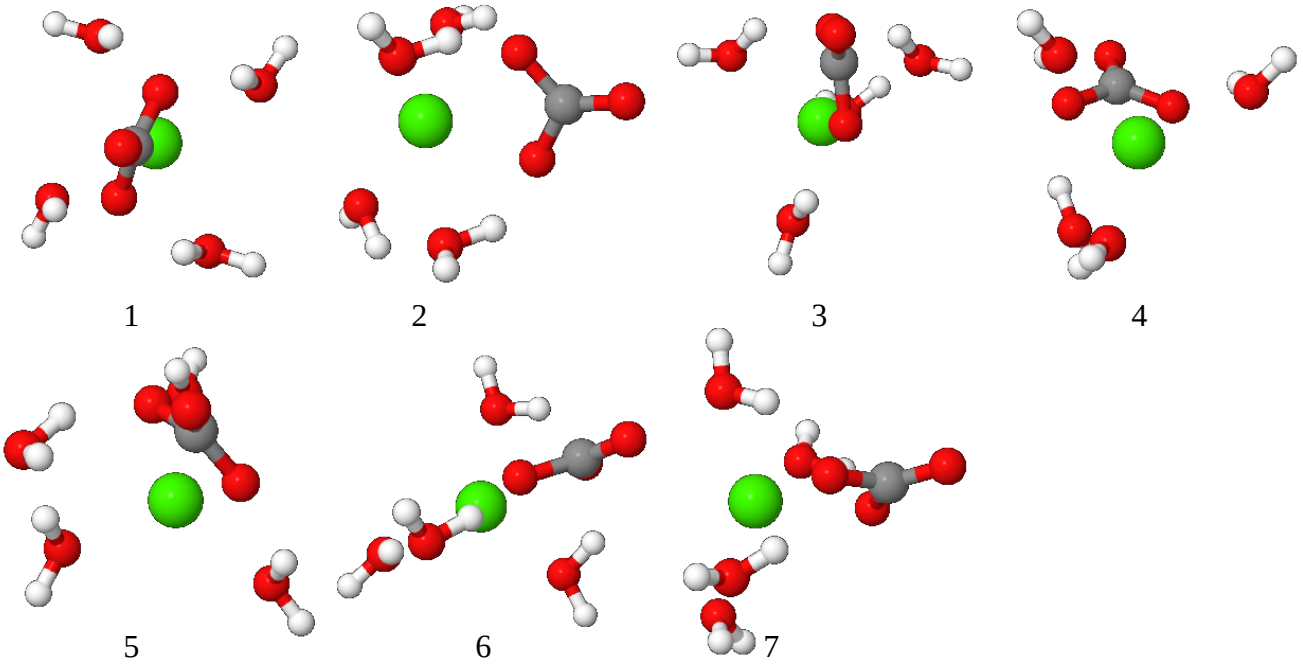

Fig. S38. $CaCO_3(H_2O)_4$ minima at the HF/6-31G* level of theory.

Structures in XYZ format available at DOI: 10.6084/m9.figshare.7077212
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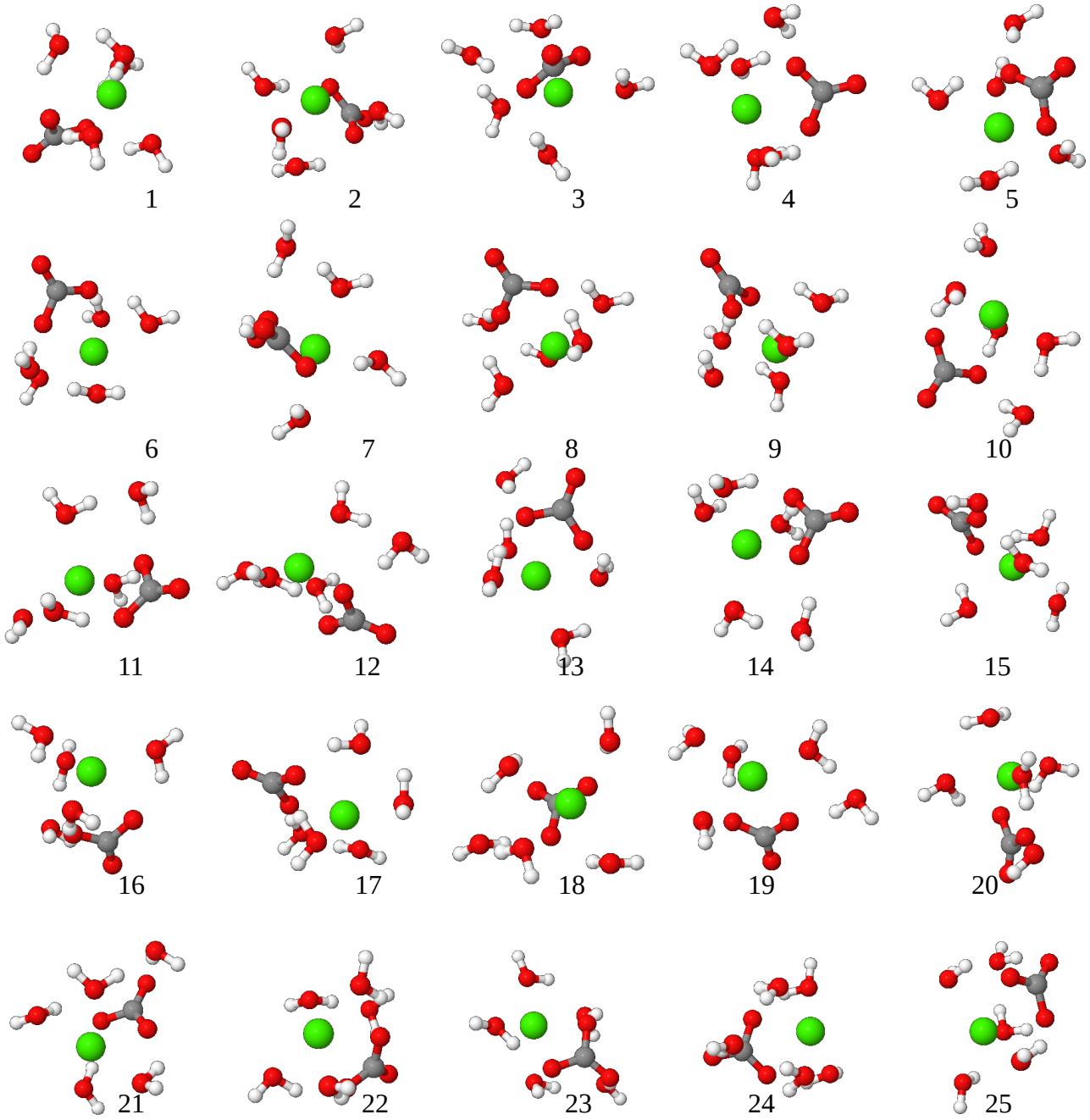

Fig. S39. $CaCO_3(H_2O)_5$ minima at the HF/6-31G* level of theory.

Structures in XYZ format available at DOI: 10.6084/m9.figshare.7077218
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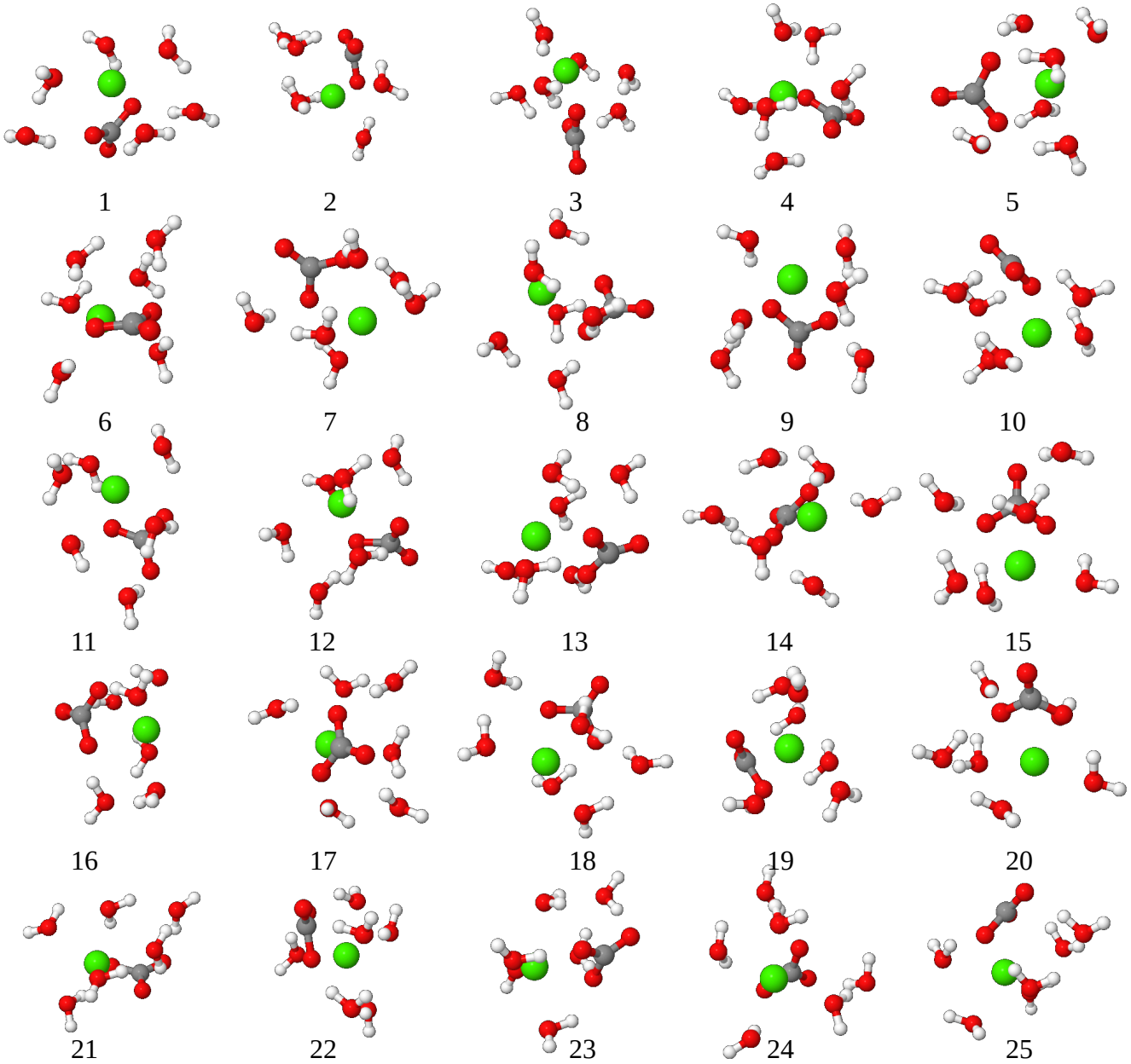

Fig. S40. $CaCO_3(H_2O)_6$ minima at the HF/6-31G* level of theory.

Structures in XYZ format available at DOI: 10.6084/m9.figshare.7077227
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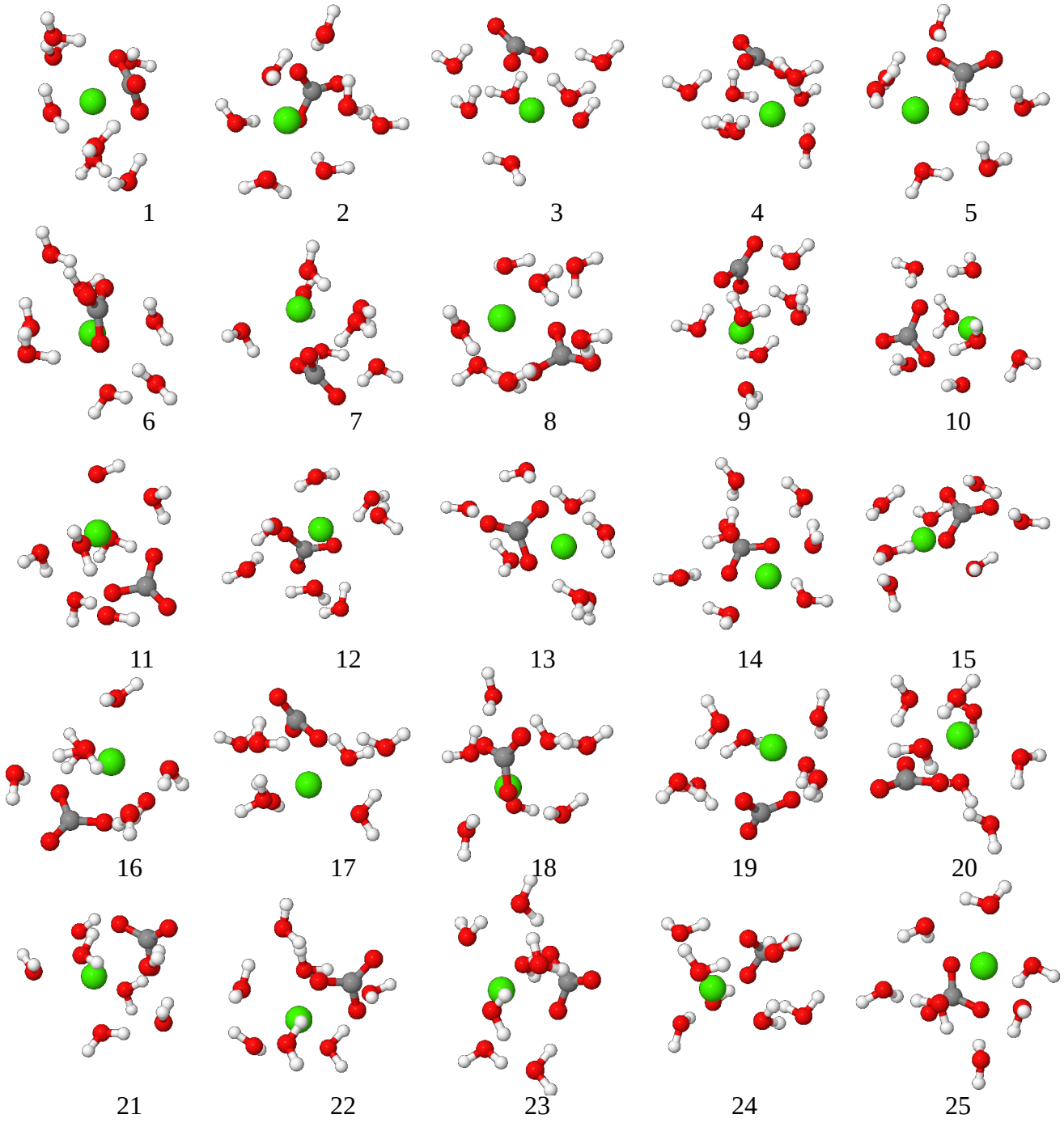

Fig. S41. $CaCO_3(H_2O)_7$ minima at the HF/6-31G* level of theory.

Structures in XYZ format available at DOI: 10.6084/m9.figshare.7077242
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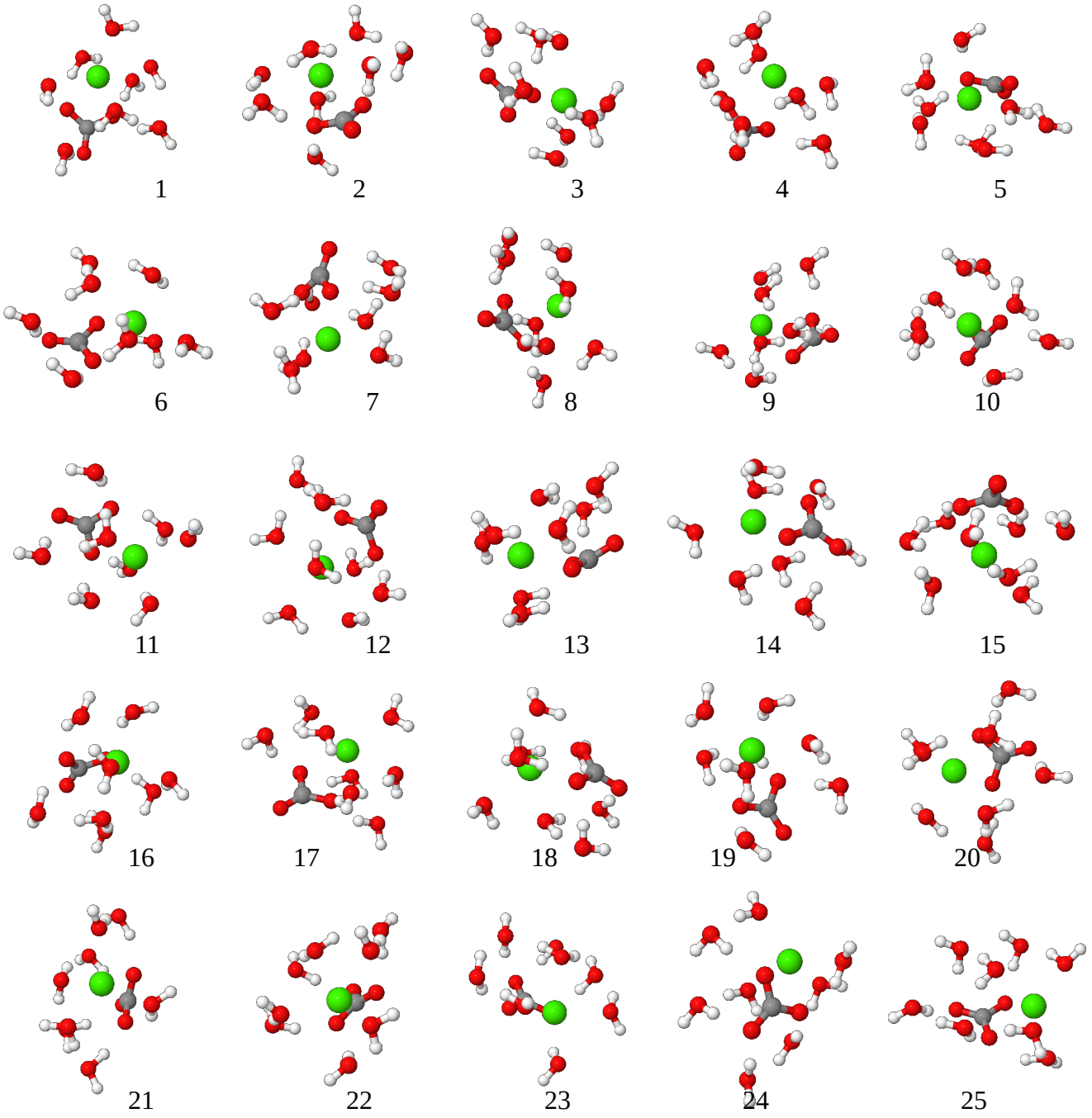

Fig. S42. $CaCO_3(H_2O)_8$ minima at the HF/6-31G* level of theory.

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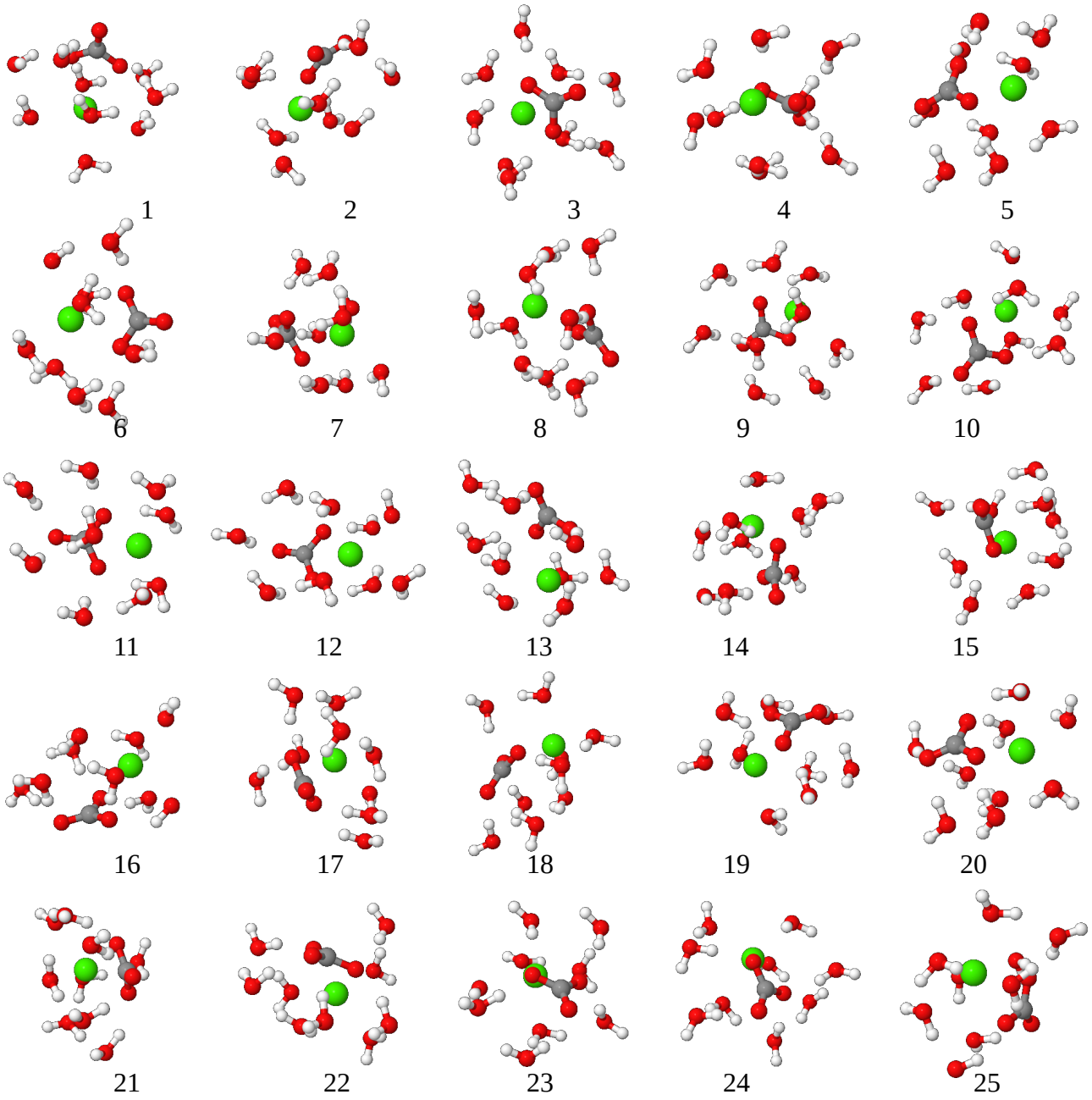

Fig. S43. $CaCO_3(H_2O)_9$ minima at the HF/6-31G* level of theory.

Structures in XYZ format available at DOI: 10.6084/m9.figshare.7077257
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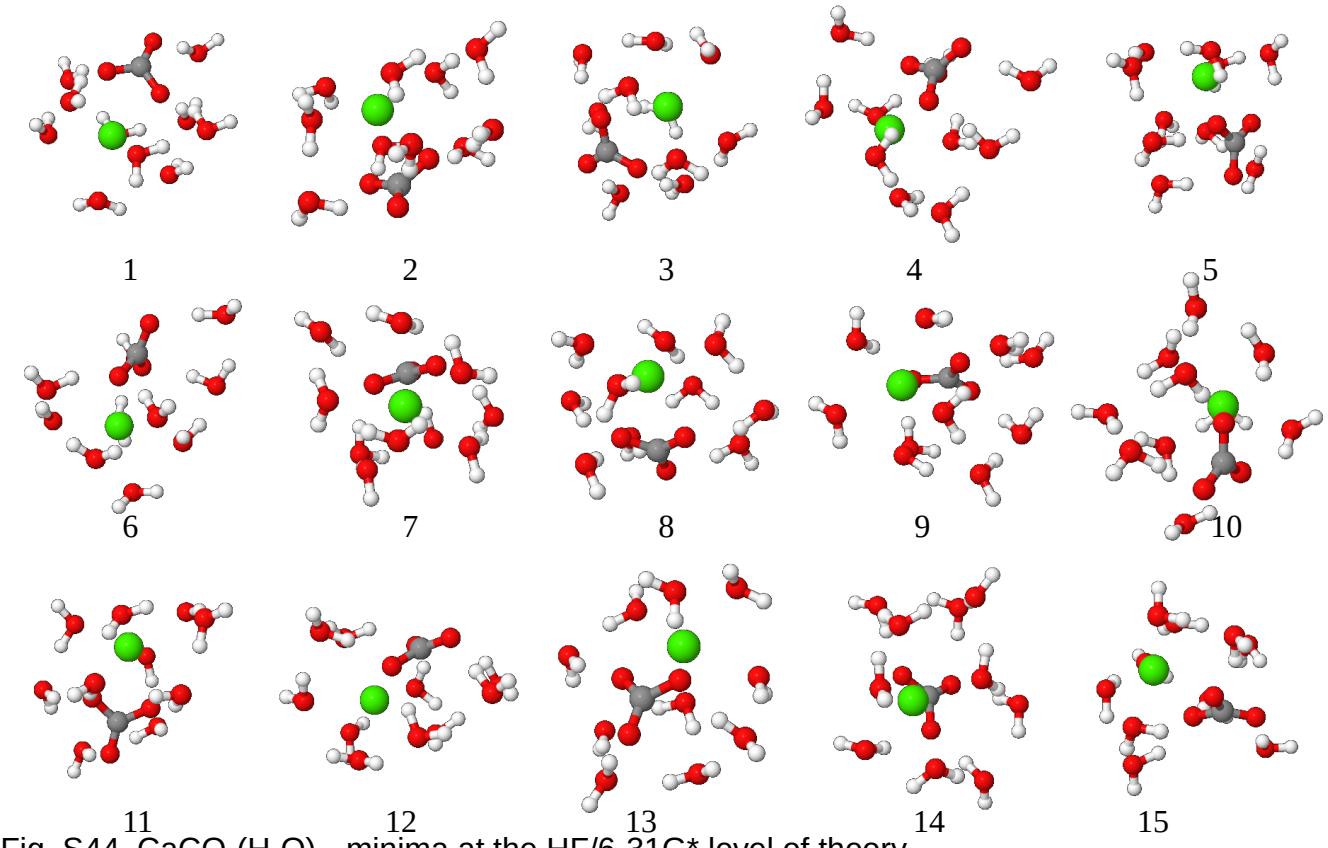

Fig. S44. $CaCO_3(H_2O)_{10}$ minima at the HF/6-31G* level of theory.

Structures in XYZ format available at DOI: 10.6084/m9.figshare.7077260
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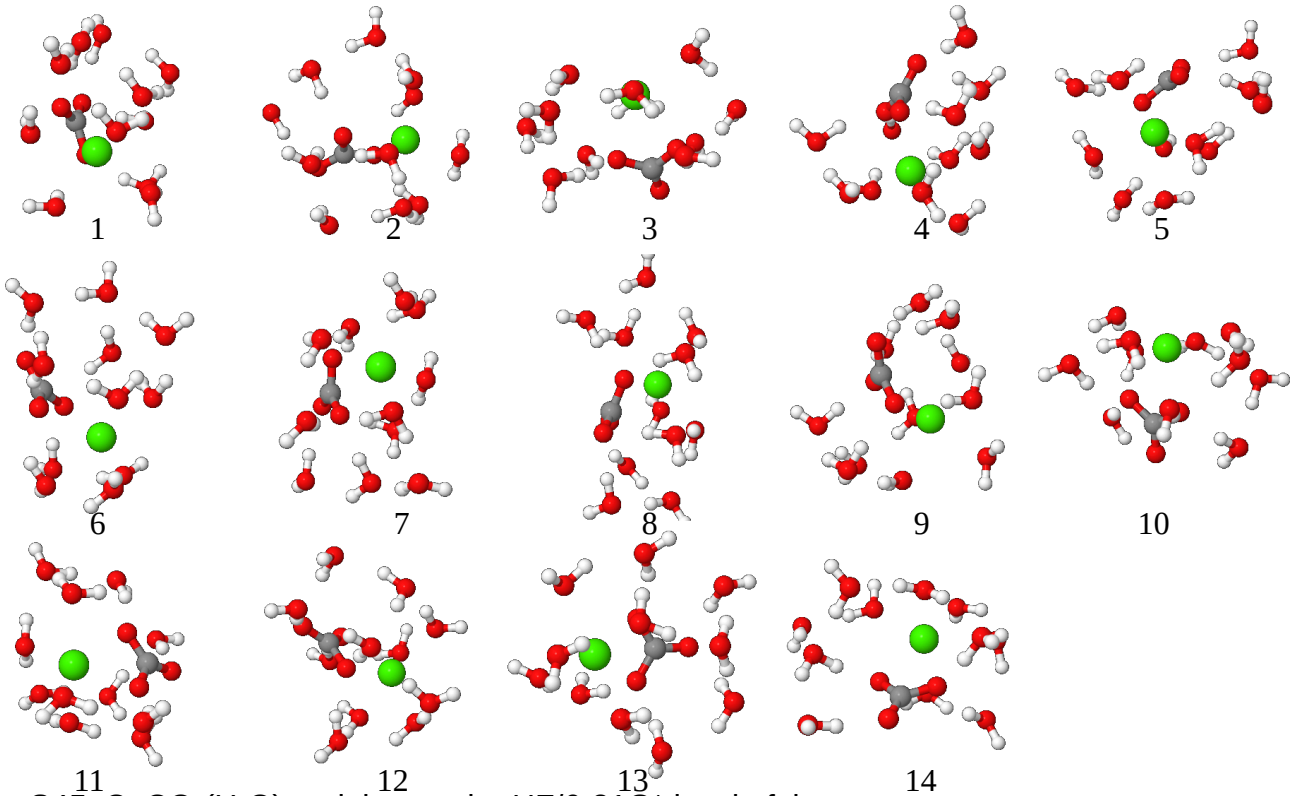

Fig. S45. $CaCO_3(H_2O)_{11}$ minima at the HF/6-31G* level of theory.

Structures in XYZ format available at DOI: 10.6084/m9.figshare.7077263
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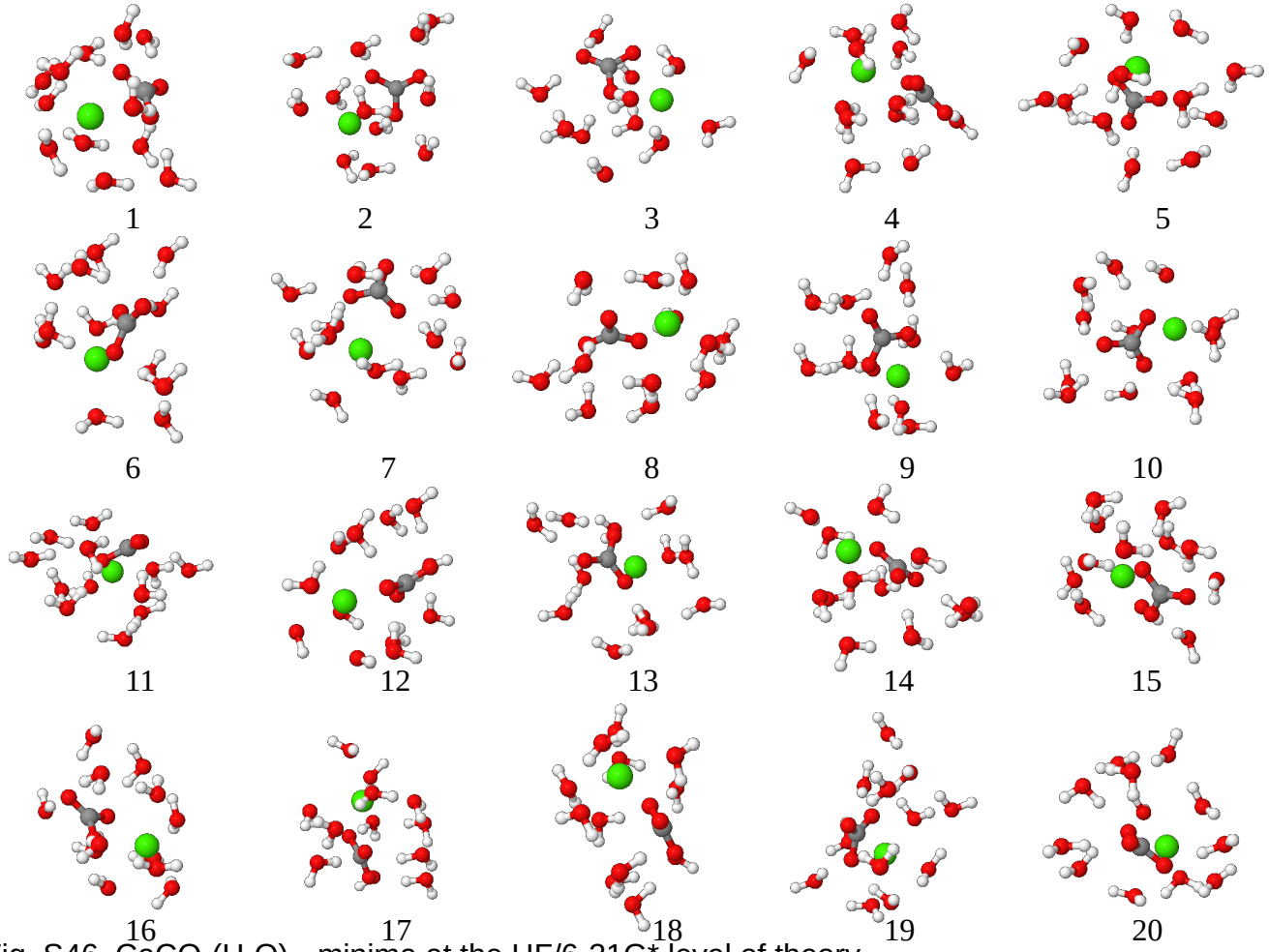

Fig. S46. $CaCO_3(H_2O)_{12}$ minima at the HF/6-31G* level of theory.

Structures in XYZ format available at DOI: 10.6084/m9.figshare.7077266
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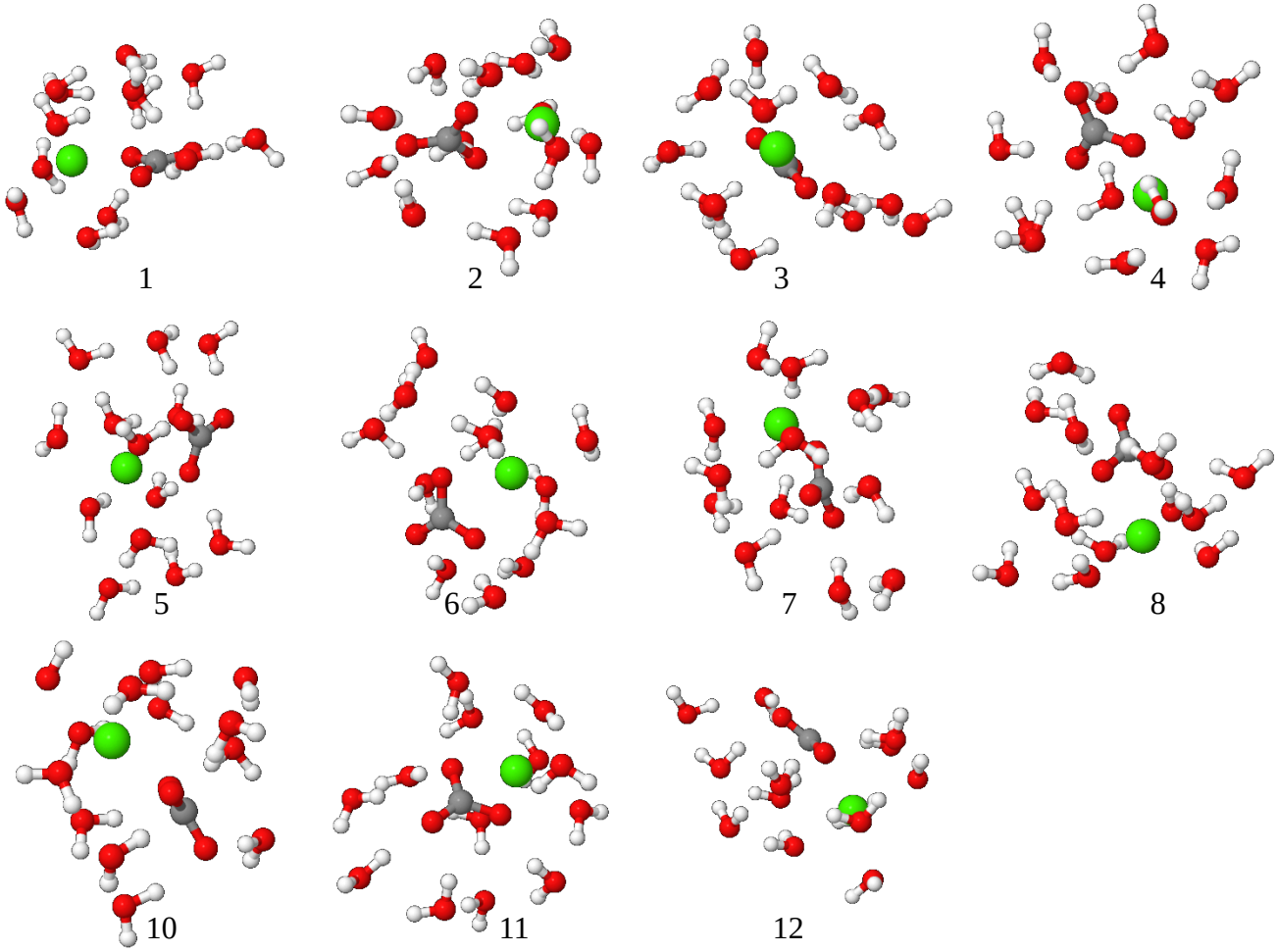

Fig. S47. $CaCO_3(H_2O)_{13}$ minima at the HF/6-31G* level of theory.

Structures in XYZ format available at DOI: 10.6084/m9.figshare.7077269
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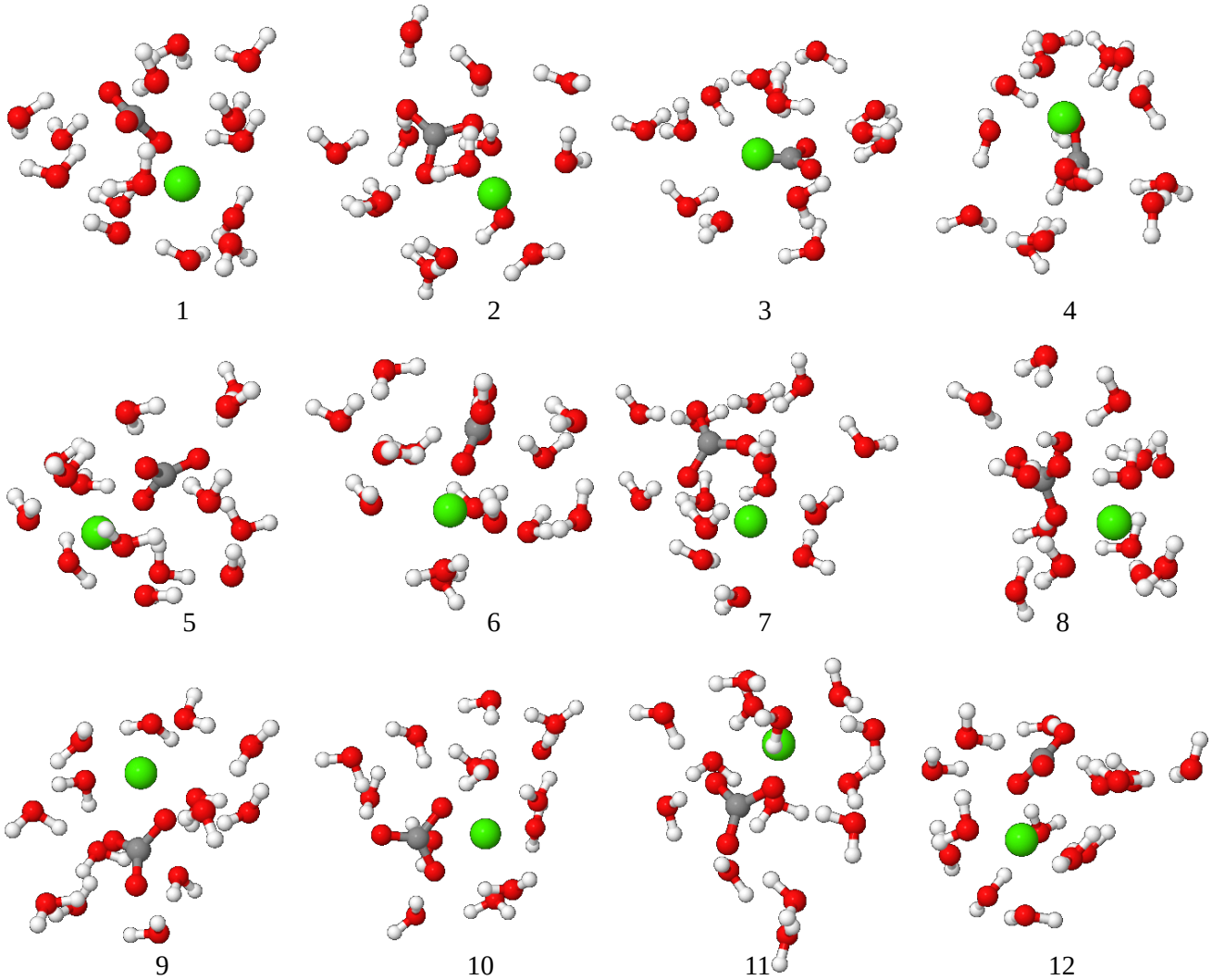

Fig. S48. $CaCO_3(H_2O)_{14}$ minima at the HF/6-31G* level of theory.

Structures in XYZ format available at DOI: 10.6084/m9.figshare.7077281
https://figshare.com/s/f82d1f9c3c2b08b56762

Table S1. Values of q_bind parameters for hydrated clusters.

Compound	ΔE/ (kcal mol^{-1})	q_bind		
		global minimum	high-energy	Δqbind
$F^-(H_2O)_6$	1.53	5.32E-04	1.88E-04	−3.44E-04
$F^-(H_2O)_7$	1.63	4.67E-04	2.57E-04	−2.10E-04
$F^-(H_2O)_8$	2.95	5.32E-05	−1.71E-05	−7.03E-05
$F^-(H_2O)_9$	1.81	5.06E-04	8.45E-04	3.39E-04
$F^-(H_2O)_{10}$	1.49	4.50E-04	2.24E-04	−2.26E-04
$CO_3^{2-}(H_2O)_5$	0.88	1.36E-03	2.85E-04	−1.07E-03
$CO_3^{2-}(H_2O)_6$	0.41	3.59E-05	2.02E-05	−1.58E-05
$CO_3^{2-}(H_2O)_7$	1.34	8.15E-04	−1.06E-03	−1.87E-03
$CO_3^{2-}(H_2O)_8$	1.24	5.02E-04	−4.73E-04	−9.75E-04
$CO_3^{2-}(H_2O)_9$	1.33	2.67E-04	−2.19E-04	−4.86E-04
$CO_3^{2-}(H_2O)_{10}$	1.00	2.69E-04	−4.27E-04	−6.96E-04
$CaF_2(H_2O)_5$	1.00	2.98E-04	2.07E-04	−9.10E-05
$CaF_2(H_2O)_6$	0.54	5.70E-04	9.52E-04	3.82E-04
$CaF_2(H_2O)_7$	2.78	1.21E-03	−1.73E-03	−2.94E-03
$CaF_2(H_2O)_8$	1.57	1.36E-03	4.89E-04	−8.69E-04
$CaF_2(H_2O)_9$	0.88	1.09E-03	1.16E-03	7.30E-05
$CaF_2(H_2O)_{10}$	0.91	1.17E-03	1.32E-03	1.48E-04
$CaF_2(H_2O)_{11}$	1.99	−1.24E-03	1.06E-03	2.30E-03
$CaF_2(H_2O)_{12}$	1.73	1.12E-03	6.14E-05	−1.06E-03
$CaF_2(H_2O)_{13}$	0.71	4.57E-04	−2.31E-04	−6.88E-04
$CaF_2(H_2O)_{14}$	2.69	1.14E-03	−1.89E-04	−1.32E-03
$CaCO_3(H_2O)_5$	1.43	4.02E-04	−5.48E-04	−9.50E-04
$CaCO_3(H_2O)_6$	1.05	1.60E-03	8.31E-04	−7.72E-04
$CaCO_3(H_2O)_7$	0.78	2.03E-03	2.14E-03	1.10E-04
$CaCO_3(H_2O)_8$	1.24	1.70E-03	1.41E-03	−2.89E-04
$CaCO_3(H_2O)_9$	1.48	6.11E-04	6.29E-04	1.84E-05
$CaCO_3(H_2O)_{10}$	2.68	1.55E-03	1.47E-03	−8.10E-05
$CaCO_3(H_2O)_{11}$	1.73	−1.44E-03	1.81E-03	3.24E-03
$CaCO_3(H_2O)_{12}$	2.61	−5.56E-04	−1.73E-02	−1.67E-02
$CaCO_3(H_2O)_{13}$	1.69	−1.89E-04	1.99E-03	2.17E-03
$CaCO_3(H_2O)_{14}$	1.51	6.19E-05	−9.93E-04	−1.05E-03