

《太赫兹光谱学研究 CL-20/MTNP 共晶振动特性*》的补充材料

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附录 A 结构优化后晶体参数结果

表 A1 CL-20 结构优化参数对比

Table A1. Comparison of structure optimization parameters for CL-20.

| 原始参数 | 默认 $s_R=1.055$ | | $s_R=1$ | |
|----------------|----------------|---------|---------|-------|
| | 优化结果 | 偏差/% | 优化结果 | 偏差/% |
| Angle α | 90 | 90 | 90 | 0.00 |
| Angle β | 106.87 | 107.817 | 107.626 | 0.71 |
| Angle γ | 90 | 90 | 90 | 0.00 |
| Volume V | 1426.97 | 1446.68 | 1415.4 | -0.81 |
| Length a | 8.855 | 8.94305 | 8.85271 | -0.03 |
| Length b | 12.579 | 12.6759 | 12.5339 | -0.36 |
| Length c | 13.387 | 13.4046 | 13.3845 | -0.02 |

表 A2 MTNP 结构优化参数对比

Table A2. Comparison of structure optimization parameters for MTNP.

| 原始参数 | 默认 $s_R=1.055$ | | $s_R=1$ | |
|----------------|----------------|---------|---------|-------|
| | 优化结果 | 偏差/% | 优化结果 | 偏差/% |
| Angle α | 90 | 90 | 90 | 0.00 |
| Angle β | 90 | 90 | 90 | 0.00 |
| Angle γ | 90 | 90 | 90 | 0.00 |
| Volume V | 842.61 | 817.172 | 837.136 | -0.65 |
| Length a | 11.9211 | 11.7991 | 11.8769 | -0.37 |
| Length b | 8.3391 | 8.26914 | 8.30592 | -0.40 |
| Length c | 8.476 | 8.37541 | 8.48605 | 0.12 |

表 A3 CL-20/MTNP 结构优化参数对比

Table A3. Comparison of structure optimization parameters for CL-20/MTNP.

| | 原始参数 | 默认 $s_R = 1.055$ | |
|----------------|---------|------------------|-------|
| | | 优化结果 | 偏差/% |
| Angle α | 90 | 90 | 0.00 |
| Angle β | 98.639 | 98.6971 | 0.06 |
| Angle γ | 90 | 90 | 0.00 |
| Volume V | 1126.95 | 1128.34 | 0.12 |
| Length a | 8.3536 | 8.32068 | -0.39 |
| Length b | 11.4249 | 11.4805 | 0.49 |
| Length c | 11.9436 | 11.9493 | 0.05 |

附录 B 三种分子振动模式分解结果

表 B1 CL-20 振动分解结果

Table B1. CL-20 vibrational decomposition results.

| 基团 | 振动频率/分子间振动 | | | | | | | 平均 |
|--------|------------|------|------|------|------|------|------|-----|
| | 0.88 | 1.33 | 1.43 | 2.07 | 2.68 | 2.75 | 3.48 | |
| 笼形骨架/% | 35.9 | 44.3 | 45.3 | 41.9 | 42.3 | 44.9 | 39.7 | 42 |
| 1-硝基/% | 6.6 | 4.8 | 2.7 | 4 | 5.7 | 2.6 | 1.5 | 4 |
| 2-硝基/% | 4.7 | 4.2 | 2.3 | 1.9 | 5.6 | 2 | 9.6 | 4.3 |
| 3-硝基/% | 9.4 | 1.7 | 2.1 | 4.6 | 5.1 | 4.3 | 0.7 | 4 |
| 4-硝基/% | 3.5 | 1.7 | 2.7 | 3 | 2.9 | 4.5 | 4 | 3.2 |
| 5-硝基/% | 2.4 | 5.9 | 1.9 | 4.2 | 2.1 | 0.9 | 6.4 | 3.4 |
| 6-硝基/% | 10.1 | 1.5 | 2 | 8.2 | 7.8 | 2 | 5.9 | 5.3 |
| 基团 | 振动频率/分子内振动 | | | | | | | 平均 |
| | 0.88 | 1.33 | 1.43 | 2.07 | 2.68 | 2.75 | 3.48 | |
| 笼形骨架/% | 3.5 | 7.9 | 9.1 | 6.5 | 6.1 | 8.6 | 5.7 | 6.8 |
| 1-硝基/% | 1.5 | 2.6 | 4.7 | 4.3 | 2.5 | 5.1 | 7.6 | 4 |
| 2-硝基/% | 3.9 | 3.5 | 5.4 | 7.2 | 2.6 | 6 | 3.3 | 4.6 |
| 3-硝基/% | 2.4 | 6.8 | 5.5 | 3.4 | 3.2 | 2.9 | 8.8 | 4.7 |
| 4-硝基/% | 5.6 | 6.8 | 4.8 | 5.6 | 6.3 | 2.6 | 4.2 | 5.1 |
| 5-硝基/% | 7.1 | 1.1 | 5.9 | 3.9 | 7.4 | 7.5 | 1 | 4.8 |
| 6-硝基/% | 3.4 | 7.2 | 5.7 | 1.5 | 0.4 | 6.1 | 1.7 | 3.7 |

表 B2 MTNP 振动分解结果

Table B2. MTNP vibrational decomposition results.

| 基团 | 振动频率/分子间振动 | | | | | | | | 平均 |
|--------|------------|------|------|------|------|------|------|------|------|
| | 0.53 | 0.88 | 0.91 | 1.54 | 1.77 | 2.16 | 2.83 | 3.41 | |
| 吡啶环/% | 43.8 | 43.8 | 43.8 | 43.3 | 43.8 | 43.8 | 44.2 | 44.5 | 43.9 |
| 1-硝基/% | 1.6 | 0.1 | 0.2 | 0.5 | 0.6 | 0.2 | 0.1 | 0 | 0.4 |
| 2-硝基/% | 0.1 | 0.3 | 0.2 | 1 | 0.2 | 0.2 | 0.1 | 0.2 | 0.3 |
| 3-硝基/% | 0.2 | 0.4 | 0.2 | 1.6 | 0.2 | 0.3 | 0.1 | 0.4 | 0.4 |
| 1-甲基/% | 0.7 | 0.3 | 0.2 | 0.4 | 0.2 | 0.2 | 0.7 | 1.3 | 0.5 |

| 基团 | 振动频率/分子间振动 | | | | | | | | 平均 |
|--------|------------|------|------|------|------|------|------|------|------|
| | 0.53 | 0.88 | 0.91 | 1.54 | 1.77 | 2.16 | 2.83 | 3.41 | |
| 吡啶环/% | 20.4 | 20.7 | 20.8 | 20 | 20.7 | 20.7 | 21 | 20.9 | 20.7 |
| 1-硝基/% | 7.8 | 8.9 | 8.8 | 8.9 | 8.4 | 8.7 | 9 | 9.2 | 8.7 |
| 2-硝基/% | 9.2 | 8.7 | 8.7 | 8.4 | 8.9 | 8.8 | 9 | 9.1 | 8.8 |
| 3-硝基/% | 9.1 | 8.6 | 8.7 | 7.9 | 8.8 | 8.6 | 9 | 8.9 | 8.7 |
| 1-甲基/% | 7.1 | 8.1 | 8.3 | 8.1 | 8.3 | 8.5 | 7 | 5.5 | 7.6 |

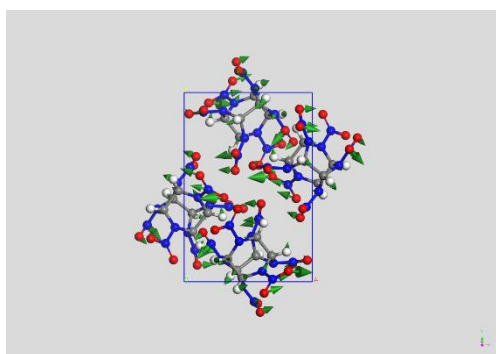
表 B3 CL-20/MTNP 振动分解结果

Table B3. CL-20/MTNP vibrational decomposition results.

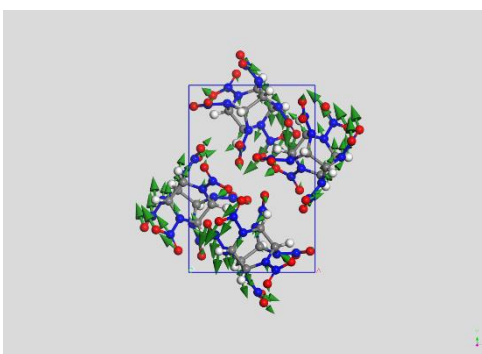
| 基团 | 振动频率/分子间振动 | | | | | | | | 平均 |
|--------|------------|------|------|------|------|------|------|------|------|
| | 0.92 | 1.26 | 1.57 | 1.97 | 2.24 | 2.54 | 3.08 | 3.4 | |
| 笼形骨架/% | 41.9 | 33 | 38.8 | 39.3 | 32.1 | 38 | 40.1 | 43.5 | 38.3 |
| 1-硝基/% | 2.7 | 3.3 | 1.7 | 1.7 | 4.2 | 2.3 | 1.6 | 1.4 | 2.4 |
| 2-硝基/% | 1.4 | 4 | 2.4 | 1.3 | 2.3 | 1.8 | 1.9 | 1.2 | 2 |
| 3-硝基/% | 1.1 | 2.1 | 3.3 | 1.2 | 8.2 | 3.9 | 2.1 | 0.7 | 2.8 |
| 4-硝基/% | 1.6 | 2.3 | 1.9 | 2.7 | 1.8 | 1.5 | 1.4 | 0.8 | 1.7 |
| 5-硝基/% | 2.7 | 1 | 0.8 | 1.5 | 1.7 | 4.8 | 3 | 0.7 | 2 |
| 6-硝基/% | 2.4 | 3.4 | 2 | 3.4 | 1.9 | 2.9 | 2.3 | 0.7 | 2.4 |
| 吡啶环/% | 0.9 | 6.6 | 5.7 | 5.9 | 5.7 | 2.6 | 1.4 | 0.8 | 3.7 |
| 1-硝基/% | 0.3 | 2.7 | 1.3 | 2.3 | 3.2 | 4 | 2.2 | 0.8 | 2.1 |
| 2-硝基/% | 0.4 | 4.5 | 3.5 | 1.3 | 2.1 | 3.2 | 1.2 | 0.5 | 2.1 |
| 3-硝基/% | 0.6 | 6.5 | 1.8 | 1.4 | 2.3 | 2.1 | 3 | 1.1 | 2.3 |
| 1-甲基/% | 0.2 | 0.7 | 1.1 | 1 | 0.9 | 1.2 | 0.3 | 0.2 | 0.7 |

| 基团 | 振动频率/分子内振动 | | | | | | | | 平均 |
|--------|------------|------|------|------|------|------|------|------|-----|
| | 0.92 | 1.26 | 1.57 | 1.97 | 2.24 | 2.54 | 3.08 | 3.4 | |
| 笼形骨架/% | 9.4 | 5.3 | 7.7 | 8 | 5.3 | 7.1 | 8.5 | 10.3 | 7.7 |
| 1-硝基/% | 1.5 | 1.9 | 3.4 | 3.3 | 0.6 | 2.9 | 3.2 | 2.7 | 2.4 |
| 2-硝基/% | 3.1 | 1.1 | 2.5 | 3.7 | 2.8 | 3.5 | 2.8 | 2.9 | 2.8 |
| 3-硝基/% | 3.4 | 3.4 | 1.4 | 3.8 | 4.2 | 1.1 | 2.5 | 3.5 | 2.9 |
| 4-硝基/% | 2.8 | 3.1 | 3.2 | 2 | 3.4 | 3.9 | 3.4 | 3.5 | 3.2 |
| 5-硝基/% | 1.5 | 4.6 | 4.4 | 3.5 | 3.5 | 0 | 1.4 | 3.6 | 2.8 |
| 6-硝基/% | 1.8 | 1.8 | 3 | 1.2 | 3.3 | 2.2 | 2.3 | 3.5 | 2.4 |
| 吡啶环/% | 3.9 | 0.3 | 0.5 | 0.2 | 0.6 | 3.5 | 3.8 | 3.7 | 2.1 |
| 1-硝基/% | 4.3 | 2.7 | 3.8 | 2.5 | 1.8 | 1 | 2.4 | 3.4 | 2.7 |
| 2-硝基/% | 4.2 | 0.5 | 1.2 | 3.7 | 3 | 1.9 | 3.7 | 3.8 | 2.7 |
| 3-硝基/% | 3.9 | 1.9 | 3.2 | 3.6 | 2.8 | 3.2 | 1.5 | 3.1 | 2.9 |
| 1-甲基/% | 4.1 | 3.4 | 1.4 | 1.6 | 2.3 | 1.3 | 4.1 | 3.7 | 2.7 |

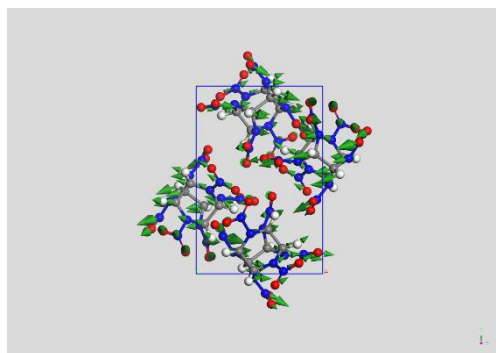
附录 C DFT 计算的振动模式



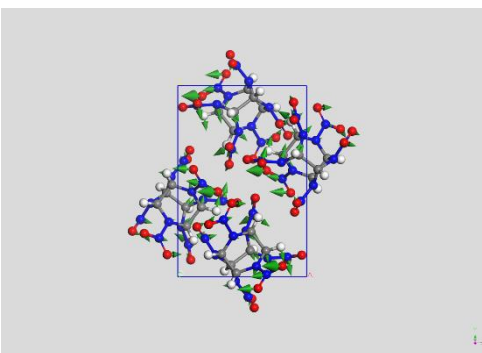
(a)



(b)



(c)



(d)

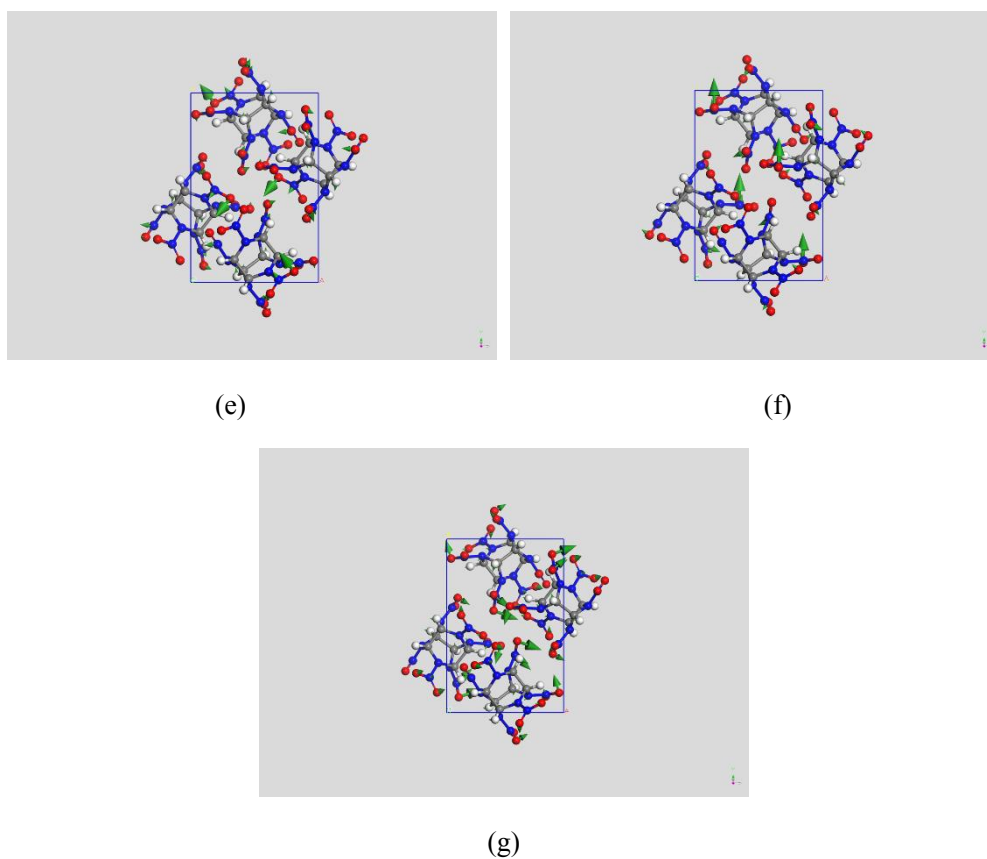
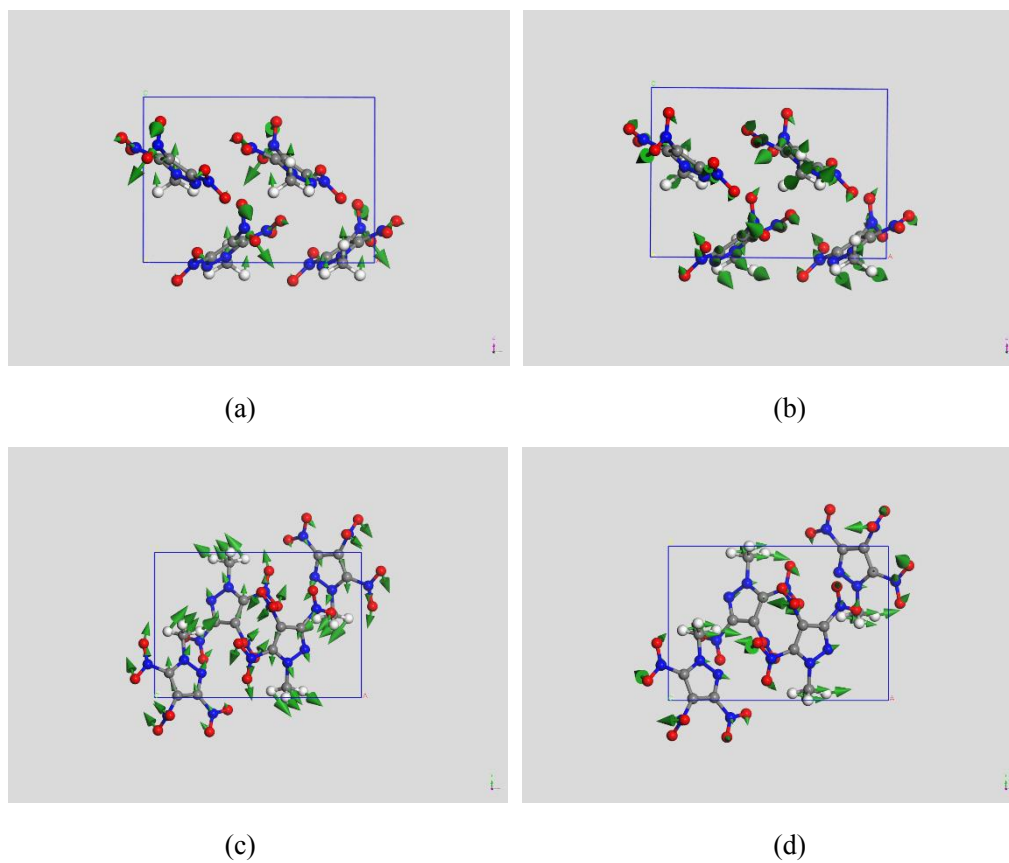


图 C1 CL-20 振动模式 (a) 0.88; (b) 1.33; (c) 1.43; (d) 2.07; (e) 2.68; (f) 2.75; (g) 3.48

Fig. C1. CL-20 vibration mode: (a) 0.88; (b) 1.33; (c) 1.43; (d) 2.07; (e) 2.68; (f) 2.75; (g) 3.48.



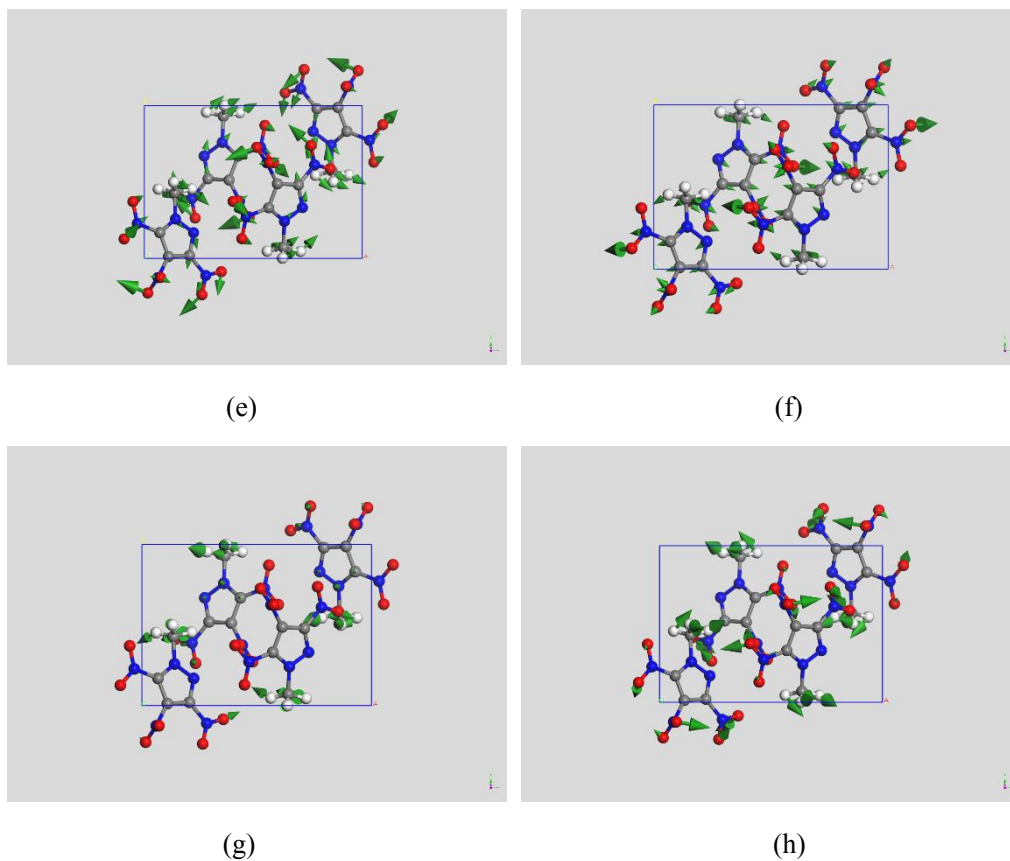
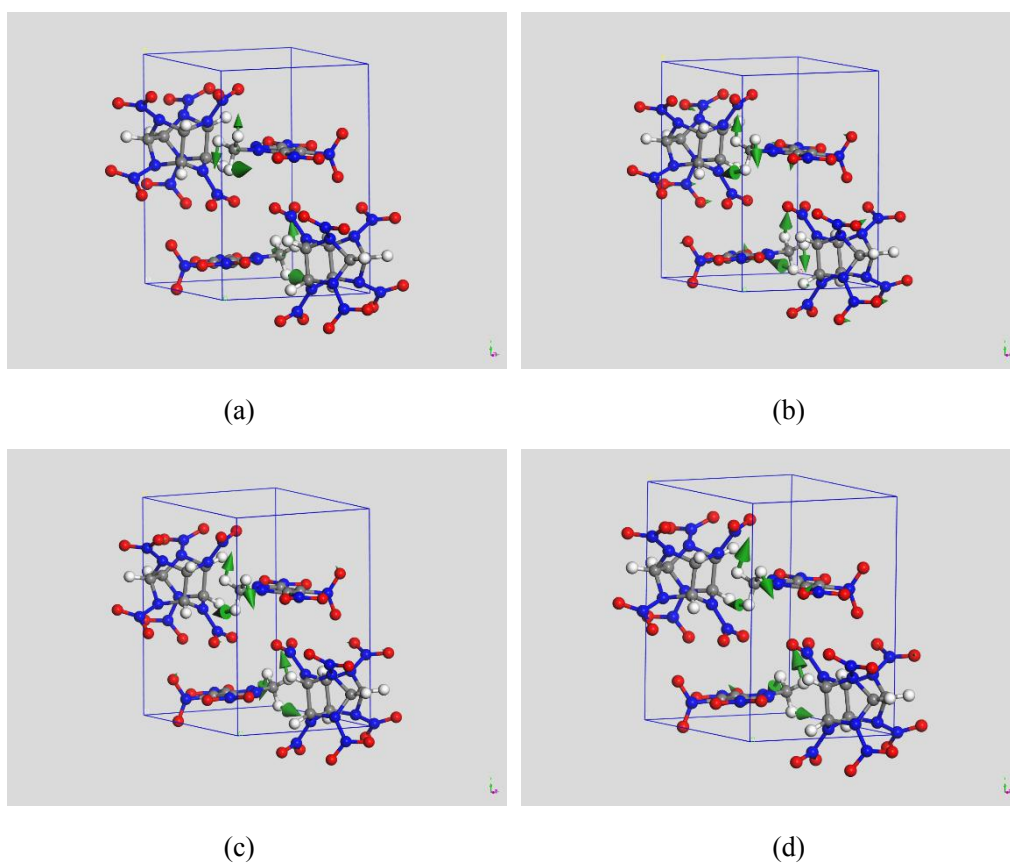


图 C2 MTNP 振动模式 (a) 0.53; (b) 0.88; (c) 0.91; (d) 1.54; (e) 1.77; (f) 2.16; (g) 2.83; (h) 3.41

Fig. C2. MTNP vibration mode: (a) 0.53; (b) 0.88; (c) 0.91; (d) 1.54; (e) 1.77; (f) 2.16; (g) 2.83; (h) 3.41.



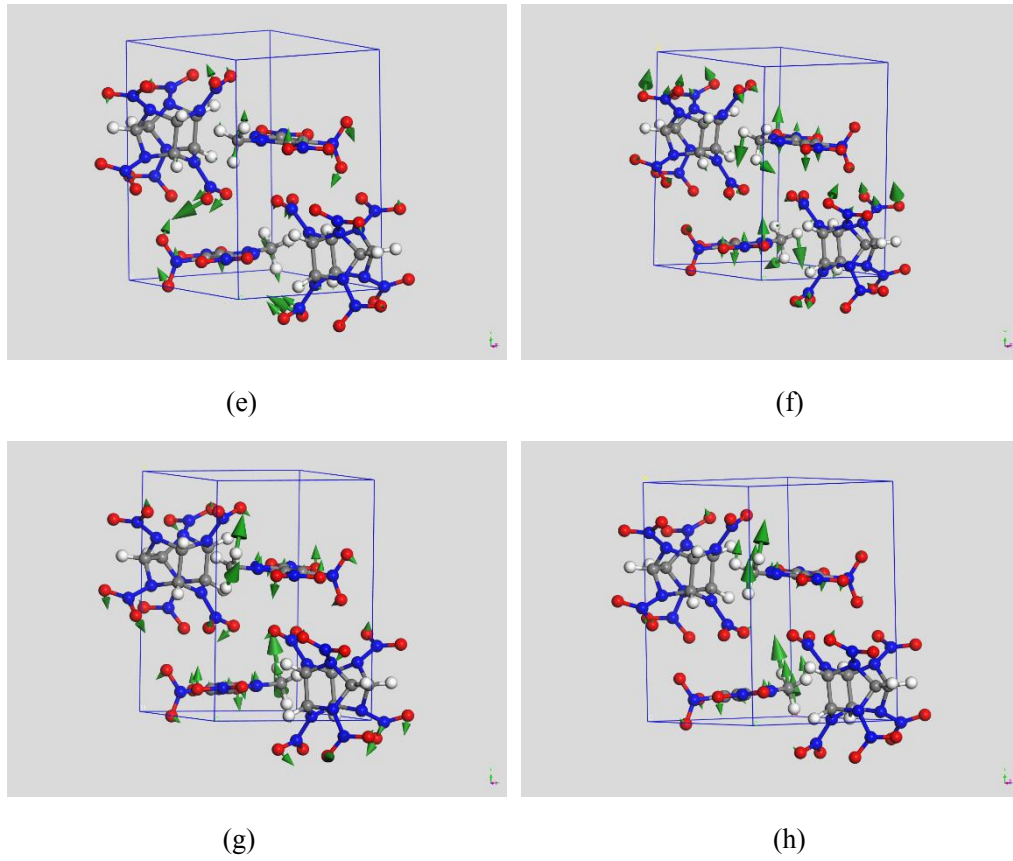


图 C-3 CL -20/MTNP 振动模式 (a) 0.92; (b) 1.26; (c) 1.57; (d) 1.97; (e) 2.24; (f) 2.54; (g) 3.08; (h) 3.40

Fig. C3. CL -20/MTNP vibration mode: (a) 0.92; (b) 1.26; (c) 1.57; (d) 1.97; (e) 2.24; (f) 2.54; (g) 3.08; (h) 3.40.